10/681,924a 4/4/05 Structure searches 1-7 (excerpts)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 APR 2005 HIGHEST RN 847818-85-3
DICTIONARY FILE UPDATES: 1 APR 2005 HIGHEST RN 847818-85-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

****

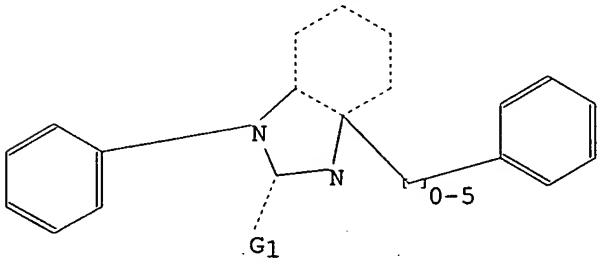
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, ADERL, is now *
* available and contains the CA role and document type information. *

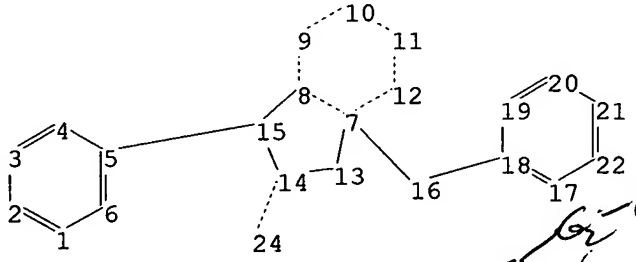
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10681924a.str

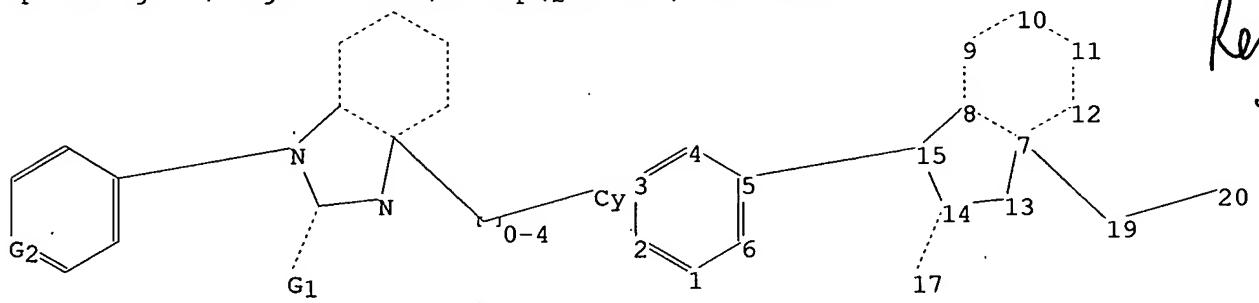




chain nodes :
16 24
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 17 18 19 20 21 22
chain bonds :
5-15 7-16 14-24 16-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14 14-15 17-18 17-22 18-19 19-20 20-21 21-22
exact/norm bonds :
5-15 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14 14-15 14-24
exact bonds :
7-16 16-18
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22

```
G1:O,S

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:CLASS  17:Atom  18:Atom  19:Atom
20:Atom  21:Atom  22:Atom  24:CLASS



L1      STRUCTURE UPLOADED

=> s L1
SAMPLE SEARCH INITIATED 09:17:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      1 TO ITERATE

100.0% PROCESSED       1 ITERATIONS                                 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            1 TO       80
PROJECTED ANSWERS:               1 TO       80

L2            1 SEA SSS SAM L1

=> s L1 full
FULL SEARCH INITIATED 09:17:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     53 TO ITERATE

100.0% PROCESSED      53 ITERATIONS                                12 ANSWERS
SEARCH TIME: 00.00.01

L3            12 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                               ENTRY    SESSION
FULL ESTIMATED COST                           161.33     161.54

FILE 'CAPLUS' ENTERED AT 09:17:46 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 4 Apr 2005  VOL 142 ISS 15
FILE LAST UPDATED: 3 Apr 2005  (20050403/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.
```

```
=> s L3
L4             1 L3

=> d L4

L4   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2005 ACS on STN
AN   2004:331928  CAPLUS
DN   140:357354
TI   A preparation of benzimidazolone derivatives useful as anti-inflammatory
     agents
IN   Dhar, T. G. Murali; Potin, Dominique; Maillet, Magali Jeannine Blandine;
     Launay, Michele; Nicolai, Eric Antoine; Iwanovicz, Edwin J.
PA   Bristol-Myers Squibb Company, USA
SO   PCT Int. Appl., 69 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
     ---------------     ----   --------    --------------------    --------
PI   WO 2004032861        A2    20040422    WO 2003-US31960         20031009
     WO 2004032861        A3    20040805
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
             TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     US 2004116467        A1    20040617    US 2003-681924          20031009
PRAI US 2002-417935P      P     20021011
OS   MARPAT 140:357354

=>
Uploading C:\Program Files\Stnexp\Queries\10681924b.str
```




```
chain nodes :
17  19  20
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15
chain bonds :
5-15  7-19  14-17  19-20
ring bonds :
```

```
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  7-13  8-9  8-15  9-10  10-11  11-12  13-14
 14-15
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-15  7-8  7-12  7-13  7-19  8-9  8-15  9-10  10-11
11-12  13-14  14-15  14-17  19-20


G1:O,S

G2:C,N

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  17:CLASS  19:CLASS  20:Atom



L5      STRUCTURE UPLOADED

=> s L5
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



SAMPLE SEARCH INITIATED 09:21:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   2176 TO ITERATE

 46.0% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        40722 TO    46318
PROJECTED ANSWERS:               0 TO        0

L6            0 SEA SSS SAM L5



L7           0 L6

=> fil reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.45     166.22

FILE 'REGISTRY' ENTERED AT 09:21:29 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:     1 APR 2005  HIGHEST RN 847818-85-3
DICTIONARY FILE UPDATES:    1 APR 2005  HIGHEST RN 847818-85-3
```

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

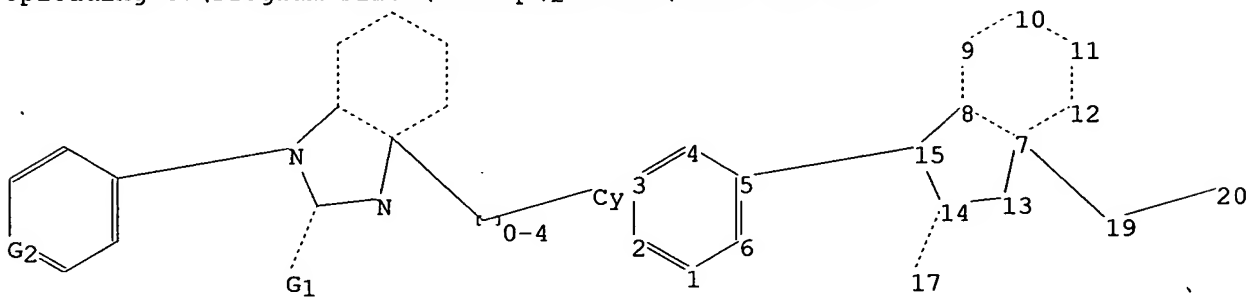
Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10681924b.str



chain nodes :
17 19 20
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
5-15 7-19 14-17 19-20
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14 14-15
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-15 7-8 7-12 7-13 7-19 8-9 8-15 9-10 10-11 11-12 13-14 14-15 14-17 19-20

G1:O,S

G2:C,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS 19:CLASS 20:Atom

```
L8      STRUCTURE UPLOADED

=> s L8 full
FULL SEARCH INITIATED 09:21:56 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  44645 TO ITERATE

100.0% PROCESSED   44645 ITERATIONS                          12 ANSWERS
SEARCH TIME: 00.00.04

L9          12 SEA SSS FUL L8

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             161.33     327.55

FILE 'CAPLUS' ENTERED AT 09:22:04 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 4 Apr 2005  VOL 142 ISS 15
FILE LAST UPDATED: 3 Apr 2005  (20050403/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

=> s L9
L10           1 L9

=> d L10

L10  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2005 ACS on STN
AN   2004:331928  CAPLUS
DN   140:357354
TI   A preparation of benzimidazolone derivatives useful as anti-inflammatory
     agents
IN   Dhar, T. G. Murali; Potin, Dominique; Maillet, Magali Jeannine Blandine;
     Launay, Michele; Nicolai, Eric Antoine; Iwanovicz, Edwin J.
PA   Bristol-Myers Squibb Company, USA
SO   PCT Int. Appl., 69 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     ---------------     ----   --------    --------------------   --------
PI   WO 2004032861        A2    20040422    WO 2003-US31960        20031009
     WO 2004032861        A3    20040805
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
```

```
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
            GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
            LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
            OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
            TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
            FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
            BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
    US 2004116467        A1    20040617    US 2003-681924        20031009
PRAI US 2002-417935P     P     20021011
OS  MARPAT 140:357354


=> fil beilstein
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                        ENTRY    SESSION
FULL ESTIMATED COST                                      1.55     329.10

FILE 'BEILSTEIN' ENTERED AT 09:22:32 ON 04 APR 2005
COPYRIGHT (c) 2005 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften
licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON February 14, 2005

FILE COVERS 1771 TO 2004.
*** FILE CONTAINS  9,133,317 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in
   separate documents and can not be searched together in one query.
   Reaction data for BEILSTEIN compounds may be displayed
   immediately with the display codes PRE (preparations) and REA
   (reactions).  A substance answer set retrieved after the search
   for a chemical name, a compounds with available reaction
   information by combining with PRE/FA, REA/FA or more generally
   with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
   between a BEILSTEIN compound and belonging reactions. For mo
   detailed reaction searches BRNs can be searched as reaction
   partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE  <<<

**********************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.                 *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE    *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE           *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                         *
* FOR PRICE INFORMATION SEE HELP COST                                 *
**********************************************************************
    NEW
* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE
  SEARCHED, SELECTED AND TRANSFERRED.
* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES,
  ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A
  COMPOUND AT A GLANCE.

=> d his

     (FILE 'HOME' ENTERED AT 09:17:06 ON 04 APR 2005)

     FILE 'REGISTRY' ENTERED AT 09:17:13 ON 04 APR 2005
L1             STRUCTURE UPLOADED
```

```
L2             1 S L1
L3            12 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 09:17:46 ON 04 APR 2005
L4             1 S L3
L5               STRUCTURE UPLOADED
                 S L5

     FILE 'REGISTRY' ENTERED AT 09:21:23 ON 04 APR 2005
L6             0 S L5

     FILE 'CAPLUS' ENTERED AT 09:21:24 ON 04 APR 2005
L7             0 S L6

     FILE 'REGISTRY' ENTERED AT 09:21:29 ON 04 APR 2005
L8               STRUCTURE UPLOADED
L9            12 S L8 FULL

     FILE 'CAPLUS' ENTERED AT 09:22:04 ON 04 APR 2005
L10            1 S L9

     FILE 'BEILSTEIN' ENTERED AT 09:22:32 ON 04 APR 2005

=> s L3
L11           0 L3

=> s L8
SAMPLE SEARCH INITIATED 09:22:55 FILE 'BEILSTEIN'
SAMPLE SCREEN SEARCH COMPLETED -     286 TO ITERATE

100.0% PROCESSED     286 ITERATIONS                                 0 ANSWERS
SEARCH TIME: 00.00.06

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          4706 TO     6734
PROJECTED ANSWERS:                0 TO        0

L12            0 SEA SSS SAM L8

=> s L9
L13            0 L9

=> fil caold
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.54     329.64

FILE 'CAOLD' ENTERED AT 09:23:16 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.  Title keywords, authors, patent
  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.
```

This file supports REGIstRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s L3
L14 0 L3

=> s L9
L15 0 L9

=> fil casreact
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.43	330.07

FILE 'CASREACT' ENTERED AT 09:23:41 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 3 Apr 2005 VOL 142 ISS 14

****
*
* CASREACT now has more than 8 million reactions *
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L3
L16 0 L3

=> s L9
L17 0 L9

=> fil reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	56.65	386.72

FILE 'REGISTRY' ENTERED AT 09:26:56 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 American Chemical Society (ACS).

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 APR 2005 HIGHEST RN 847818-85-3
DICTIONARY FILE UPDATES: 1 APR 2005 HIGHEST RN 847818-85-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

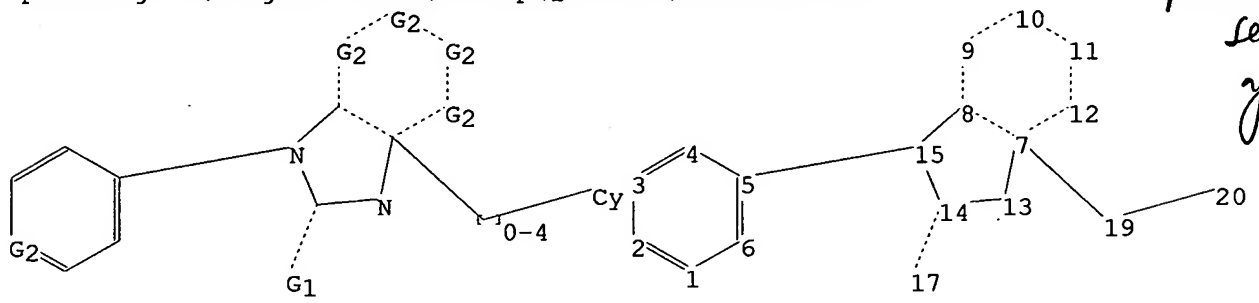
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

```
**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
**********************************************************************
```

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10681924c.str



Revise search yam

chain nodes :
17 19 20
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
5-15 7-19 14-17 19-20
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14
14-15
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-15 7-8 7-12 7-13 7-19 8-9 8-15 9-10 10-11
11-12 13-14 14-15 14-17 19-20

G1:O,S

G2:C,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS 19:CLASS 20:Atom

L18 STRUCTURE UPLOADED

```
=> s L18
SAMPLE SEARCH INITIATED 09:27:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1703 TO ITERATE

 58.7% PROCESSED    1000 ITERATIONS                                 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        31585 TO    36535
PROJECTED ANSWERS:               0 TO        0

L19           0 SEA SSS SAM L18

=> s L18 full
FULL SEARCH INITIATED 09:27:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  34288 TO ITERATE

100.0% PROCESSED   34288 ITERATIONS                              12 ANSWERS
SEARCH TIME: 00.00.03

L20          12 SEA SSS FUL L18

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             161.33     548.05

FILE 'CAPLUS' ENTERED AT 09:27:32 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 4 Apr 2005  VOL 142 ISS 15
FILE LAST UPDATED: 3 Apr 2005  (20050403/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

=> s L20
L21           1 L20

=> d L21

L21  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2005 ACS on STN
AN   2004:331928  CAPLUS
DN   140:357354
TI   A preparation of benzimidazolone derivatives useful as anti-inflammatory
     agents
```

IN Dhar, T. G. Murali; Potin, Dominique; Maillet, Magali Jeannine Blandine; Launay, Michele; Nicolai, Eric Antoine; Iwanovicz, Edwin J.
PA Bristol-Myers Squibb Company, USA
SO PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004032861	A2	20040422	WO 2003-US31960	20031009
	WO 2004032861	A3	20040805		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004116467	A1	20040617	US 2003-681924	20031009
PRAI	US 2002-417935P	P	20021011		
OS	MARPAT 140:357354				

our app

=> d L21 ibib hitstr

L21 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:331928 CAPLUS
DOCUMENT NUMBER: 140:357354
TITLE: A preparation of benzimidazolone derivatives useful as anti-inflammatory agents
INVENTOR(S): Dhar, T. G. Murali; Potin, Dominique; Maillet, Magali Jeannine Blandine; Launay, Michele; Nicolai, Eric Antoine; Iwanovicz, Edwin J.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

our app

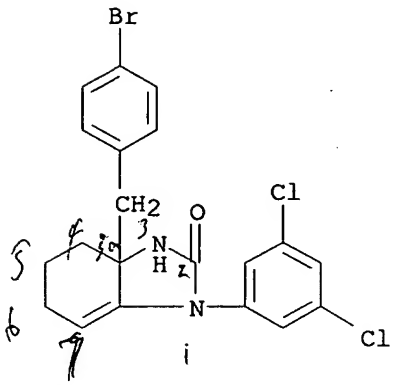
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004032861	A2	20040422	WO 2003-US31960	20031009
WO 2004032861	A3	20040805		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004116467	A1	20040617	US 2003-681924	20031009
PRIORITY APPLN. INFO.:			US 2002-417935P	P 20021011
OTHER SOURCE(S):	MARPAT 140:357354			

IT **681261-14-3P 681261-15-4P 681261-21-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of benzimidazolone derivs. useful as anti-inflammatory agents)

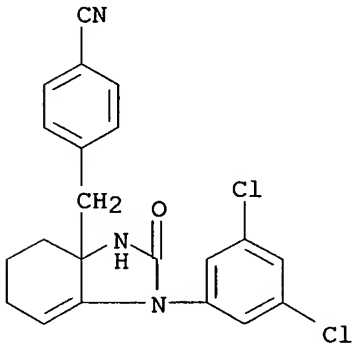
RN 681261-14-3 CAPLUS

CN 2H-Benzimidazol-2-one, 3a-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-1,3,3a,4,5,6-hexahydro- (9CI) (CA INDEX NAME)



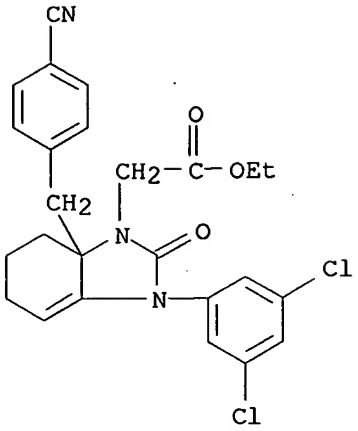
RN 681261-15-4 CAPLUS

CN Benzonitrile, 4-[[1-(3,5-dichlorophenyl)-1,2,3,4,5,6-hexahydro-2-oxo-3aH-benzimidazol-3a-yl]methyl]- (9CI) (CA INDEX NAME)



RN 681261-21-2 CAPLUS

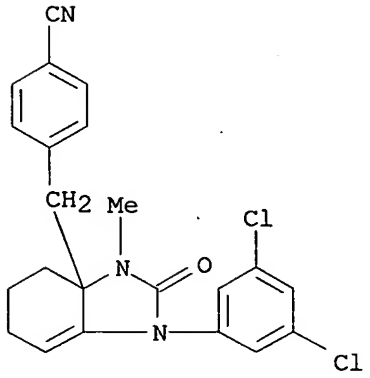
CN 1H-Benzimidazole-1-acetic acid, 7a-[(4-cyanophenyl)methyl]-3-(3,5-dichlorophenyl)-2,3,5,6,7,7a-hexahydro-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



IT **681261-16-5P 681261-17-6P 681261-18-7P**
681261-19-8P 681261-20-1P 681261-22-3P
681261-23-4P 681261-24-5P 681261-25-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzimidazolone derivs. useful as anti-inflammatory agents)

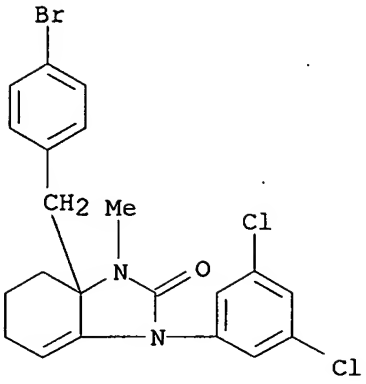
RN 681261-16-5 CAPLUS

CN Benzonitrile, 4-[[1-(3,5-dichlorophenyl)-1,2,3,4,5,6-hexahydro-3-methyl-2-oxo-3aH-benzimidazol-3a-yl]methyl]- (9CI) (CA INDEX NAME)

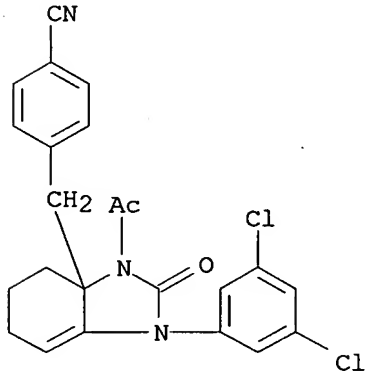


RN 681261-17-6 CAPLUS

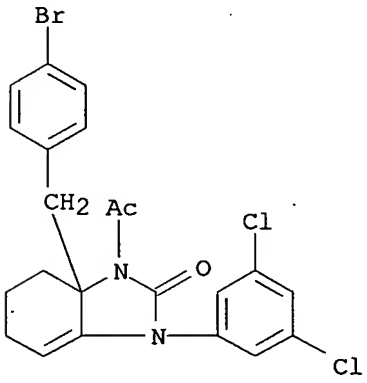
CN 2H-Benzimidazol-2-one, 3a-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-1,3,3a,4,5,6-hexahydro-3-methyl- (9CI) (CA INDEX NAME)



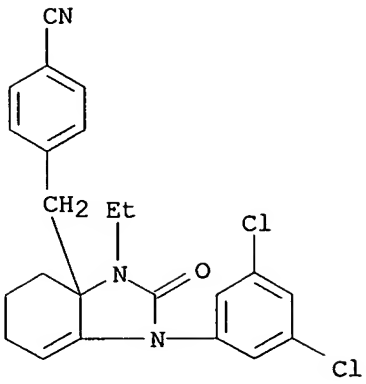
RN 681261-18-7 CAPLUS
CN 2H-Benzimidazol-2-one, 3-acetyl-3a-[(4-cyanophenyl)methyl]-1-(3,5-dichlorophenyl)-1,3,3a,4,5,6-hexahydro- (9CI) (CA INDEX NAME)



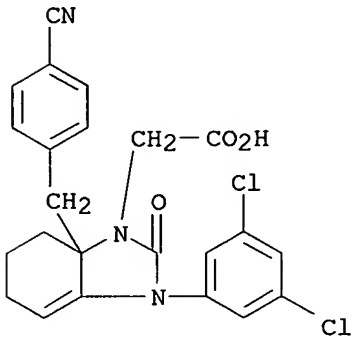
RN 681261-19-8 CAPLUS
CN 2H-Benzimidazol-2-one, 3-acetyl-3a-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-1,3,3a,4,5,6-hexahydro- (9CI) (CA INDEX NAME)



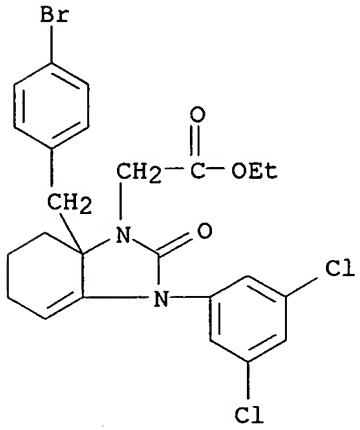
RN 681261-20-1 CAPLUS
CN Benzonitrile, 4-[[1-(3,5-dichlorophenyl)-3-ethyl-1,2,3,4,5,6-hexahydro-2-oxo-3aH-benzimidazol-3a-yl]methyl]- (9CI) (CA INDEX NAME)



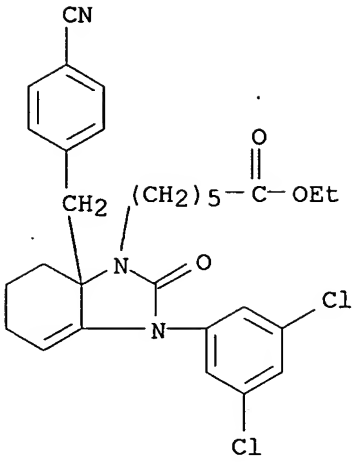
RN 681261-22-3 CAPLUS
CN 1H-Benzimidazole-1-acetic acid, 7a-[(4-cyanophenyl)methyl]-3-(3,5-dichlorophenyl)-2,3,5,6,7,7a-hexahydro-2-oxo- (9CI) (CA INDEX NAME)



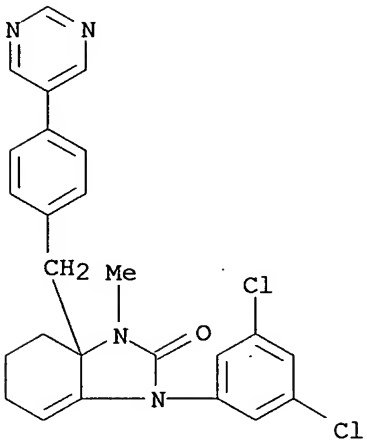
RN 681261-23-4 CAPLUS
CN 1H-Benzimidazole-1-acetic acid, 7a-[(4-bromophenyl)methyl]-3-(3,5-dichlorophenyl)-2,3,5,6,7,7a-hexahydro-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 681261-24-5 CAPLUS
CN 1H-Benzimidazole-1-hexanoic acid, 7a-[(4-cyanophenyl)methyl]-3-(3,5-dichlorophenyl)-2,3,5,6,7,7a-hexahydro-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 681261-25-6 CAPLUS
CN 2H-Benzimidazol-2-one, 1-(3,5-dichlorophenyl)-1,3,3a,4,5,6-hexahydro-3-methyl-3a-[[4-(5-pyrimidinyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	6.74	554.79

FILE 'REGISTRY' ENTERED AT 09:30:47 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 APR 2005 HIGHEST RN 847818-85-3
DICTIONARY FILE UPDATES: 1 APR 2005 HIGHEST RN 847818-85-3

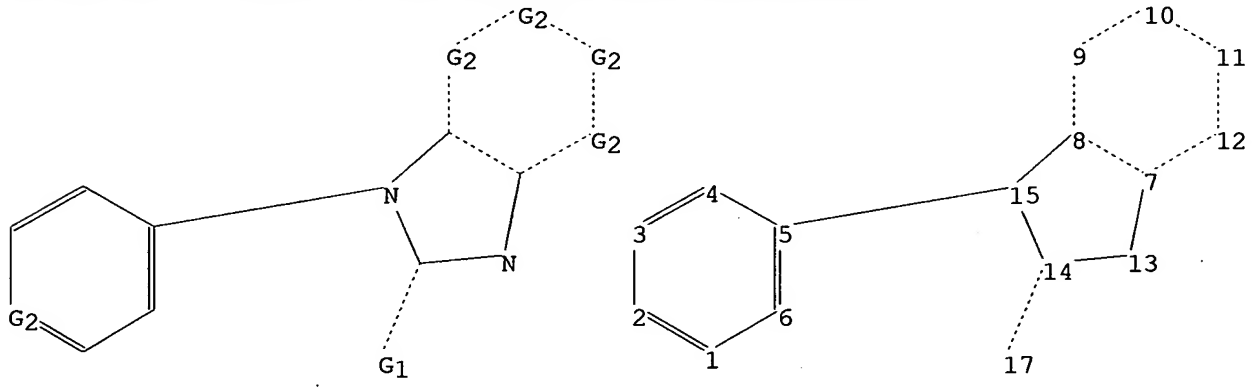
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when

conducting SmartSELECT searches.

```
**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from  *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
**********************************************************************

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10681924d.str
```

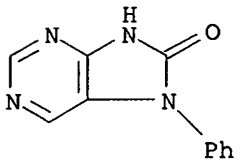
broaden search



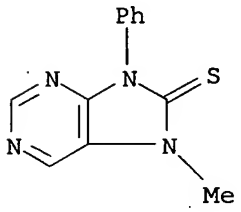

```
chain nodes :
17
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15
chain bonds :
5-15  14-17
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  7-13  8-9  8-15  9-10  10-11  11-12  13-14
 14-15
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-15  7-8  7-12  7-13  8-9  8-15  9-10  10-11  11-12
13-14  14-15  14-17


G1:O,S

G2:C,N

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  17:CLASS



L22      STRUCTURE UPLOADED
```

```
=> s L22
SAMPLE SEARCH INITIATED 09:31:08 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1703 TO ITERATE

 58.7% PROCESSED    1000 ITERATIONS                                36 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        31585 TO    36535
PROJECTED ANSWERS:             757 TO     1695

L23          36 SEA SSS SAM L22

=> s L22 full
FULL SEARCH INITIATED 09:31:16 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  34288 TO ITERATE

100.0% PROCESSED   34288 ITERATIONS                            1533 ANSWERS
SEARCH TIME: 00.00.01

L24        1533 SEA SSS FUL L22

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               161.33     716.12

FILE 'CAPLUS' ENTERED AT 09:31:20 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 4 Apr 2005  VOL 142 ISS 15
FILE LAST UPDATED: 3 Apr 2005  (20050403/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s L24
L25          438 L24

=> d ibib abs hitstr 400-438

L25  ANSWER 400 OF 438  CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         1967:473583  CAPLUS
DOCUMENT NUMBER:          67:73583
TITLE:                    Syntheses in the purine series.  XVIII.  Purine
                          syntheses with 4-amino-5-alkyl(aryl) aminopyrimidines.
                          4,5-Dihydroxypyrimidine
```

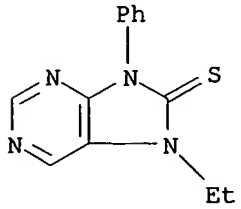
AUTHOR(S): Bredereck, Hellmut; Effenberger, Franz; Oesterlin, Hans G.
CORPORATE SOURCE: Tech. Hochsch., Stuttgart, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1967), 100(7), 2280-91
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 67:73583
GI For diagram(s), see printed CA Issue.
AB cf. CA 64: 17597b. Purines, such as 8-thioxo-7,9-disubstituted-dihydropurines (I) were prepared by treating 4-amino-5-(R-substituted-amino)pyrimidines with amidine hydrochlorides, diphenylcarbodiimide, PhNCO, isothiocyanates, or thiourea. Alkaline hydrolysis of I yielded 4,5-bis(substituted amino)pyrimidines, which reacted with urea to form 8-oxo-7,9-disubstituted-dihydropurines, and which could be further hydrolyzed to 4,5-dihydroxypyrimidines.
IT **15837-23-7P 15837-24-8P 15837-25-9P**
15837-27-1P 15837-33-9P 15837-40-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 15837-23-7 CAPLUS
CN Purin-8(9H)-one, 7-phenyl- (8CI) (CA INDEX NAME)



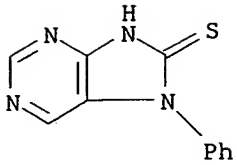
RN 15837-24-8 CAPLUS
CN Purine-8(9H)-thione, 7-methyl-9-phenyl- (8CI) (CA INDEX NAME)



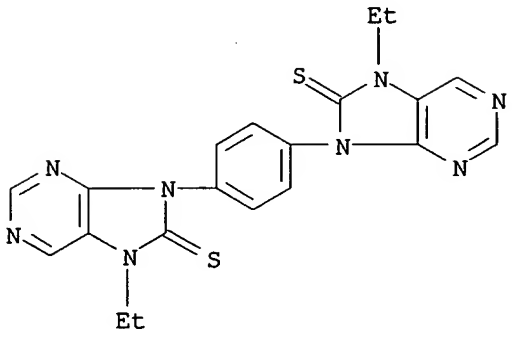
RN 15837-25-9 CAPLUS
CN Purine-8(9H)-thione, 7-ethyl-9-phenyl- (8CI) (CA INDEX NAME)



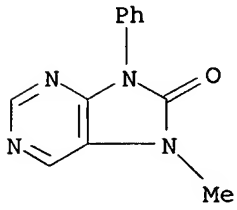
RN 15837-27-1 CAPLUS
CN Purine-8(9H)-thione, 7-phenyl- (8CI) (CA INDEX NAME)



RN 15837-33-9 CAPLUS
CN Purine-8(9H)-thione, 9,9'-p-phenylenebis[7-ethyl- (8CI) (CA INDEX NAME)



RN 15837-40-8 CAPLUS
CN Purin-8(9H)-one, 7-methyl-9-phenyl- (8CI) (CA INDEX NAME)



L25 ANSWER 401 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1967:424095 CAPLUS
DOCUMENT NUMBER: 67:24095
TITLE: Synthesis of flotation reagents and improvements in the technology of their production
AUTHOR(S): Silina, E. I.
SOURCE: Tr. Nauch.-Issled. Proekt. Inst. Obogashch. Mekh. Obrab. Polez. Iskop. Uralmekhanobr. (1965), No. 12, 273-87
From: Ref. Zh., Khim. 1967, Pt. II, Abstr. No. 5R421
DOCUMENT TYPE: Journal
LANGUAGE: Russian

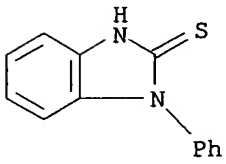
AB New reagents used for flotation of sulfide and oxidized ores of non-ferrous metals were synthesized. Special attention is given to reagent FBM (1-phenyl-2-mercaptobenzimidazole) and reagent 2Ts6D (Na di-cyclohexyldithiocarbamate). A synthetic flocculant of the polyamide type (polyacrylamide AMF) is proposed as a replacement for flour for coagulation and separation of red mud from an aluminate solution in production of Al2O3 from bauxites. Synthetic BuOH was substituted for BuOH obtained by fermentation of raw foodstuffs for production of butylxanthates. For flotation of minerals (fluorite, calcite, dolomite, etc.), a mixture of

fatty acids (reagent TZhK) can be used in place of the expensive oleic acid obtained from foodstuffs. A rapid-mixing reactor was developed for obtaining dry xanthates in which synthesis is carried out in 1 apparatus with equimolar amts. of alc., alkali, and CS2 without diluents and at relatively low temps. Waters from dredging and hydraulic processes can be clarified with Al2(SO4)3 and polyacrylamide.

IT **4493-32-7**
RL: PROC (Process)
(as flotation agent)

RN 4493-32-7 CAPLUS

CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



L25 ANSWER 402 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1967:421996 CAPLUS

DOCUMENT NUMBER: 67:21996

TITLE: Formation of complexes from azobenzenes and cyclopentadienylcobalt derivatives

AUTHOR(S): Joh, Takashi; Hagihara, Nobue; Murahashi, Shunsuke

CORPORATE SOURCE: Osaka Univ., Osaka, Japan

SOURCE: Bulletin of the Chemical Society of Japan (1967), 40(3), 661-4
CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE: English

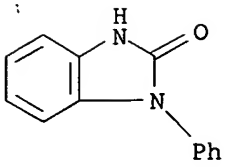
GI For diagram(s), see printed CA Issue.

AB The mixture of 5 g. (π-C5H5)Co(CO)2 (I) and 5 g. azobenzene was heated 3.5 hrs. at 160° under a N atmospheric The reaction mixture was extracted with C6H6 and chromatographed on alumina to give red-purple II, m. 162-3°. II was also prepared by heating a mixture of 5 g. (π-C5H5)2Co and 20 g. azobenzene 3.5 hrs. at 135° or by heating a mixture of 1 g. I and 1.8 g. o-aminodiphenylamine 6 hrs. at 150-60° under N. A solution of 3 g. 4,4'-dimethylazobenzene and 2.5 g. I in 30 ml. xylene was refluxed 4 hrs. and the reaction mixture chromatographed and recrystd. to yield the red-purple III, m. 172-3°. A solution of 3 g. o-phenylenediamine and 2.5 g. I in 15 ml. C6H6 was stirred at room temperature in air 20 hrs. to give IV, m. 179-80°. An Et2O solution of 1,2-diimino-3,5-cyclohexadiene and I was stirred 6 hrs. at 0° to give IV. A solution of 1 g. II in C6H6 in an autoclave was charged with CO <100 kg./cm.1 The autoclave was heated 6 hrs. at 200° under constant shaking; after cooling, C6H6 was removed, the residue washed with hexane, treated with 5% aqueous solution of NaOH, and filtered. The filtrate was acidified with HCl to precipitate wet crystalline N-phenylbenzimidazolone, m. 207-8°. A solution of 3 g. II in 50 ml. C6H6 in an autoclave was charged with 100 kg./cm.2 H, and heated 6 hrs. at 200° and the solvent removed to give o-aminodiphenylamine, m. 80-1° (C6H6). IV (55 mg.) in 20 ml. C6H6 was treated with 100 kg./cm.2 CO 4 hrs. at 200° to give I and benzimidazole. The compds. thus prepared were characterized by ir spectra.

IT **14813-85-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 14813-85-5 CAPLUS

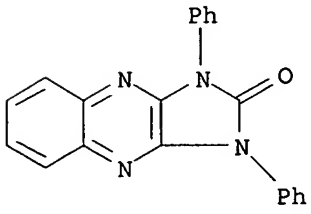
CN 2H-Benzimidazol-2-one, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



L25 ANSWER 403 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1967:403067 CAPLUS
DOCUMENT NUMBER: 67:3067
TITLE: Quinoxaline N-oxides. VII. Reaction of quinoxaline 1-oxide with phenyl isocyanate
AUTHOR(S): Iijima, Chihoko
CORPORATE SOURCE: Coll. Pharm., Shizuoka, Japan
SOURCE: Yakugaku Zasshi (1967), 87(2), 164-7
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB cf. preceding abstract Reaction of quinoxaline 1-oxide (I) with PhNCO (II) was carried out under various conditions. Thus, when I is heated with II at 80° using an oil bath or a sealed tube at 110-20° it gives 1,3-diphenyl-1-(2-quinoxalinyl)urea (III), m. 164°. III is comparatively unstable to heating and, when heated in C6H6, it gives diphenylurea and 1,3-diphenyl-1,3-bis(2-quinoxalinyl)urea (IV), m. 151.5°. Hydrolysis of IV gives 2-anilinoquinoxaline (V), yellow, m. 137° (petr. ether). When I reacts with 1.5 moles II in a sealed tube at 180° it gives V and 1,3-diphenyl-1H-imidazo[4,5-b]quinoxalin2(3H)-one (VI), m. 275-6°. VI is stable to acid hydrolysis. Using excess II in the above reaction, III is obtained besides V and VI.

IT **15051-50-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 15051-50-0 CAPLUS
CN 2H-Imidazo[4,5-b]quinoxalin-2-one, 1,3-dihydro-1,3-diphenyl- (8CI, 9CI) (CA INDEX NAME)



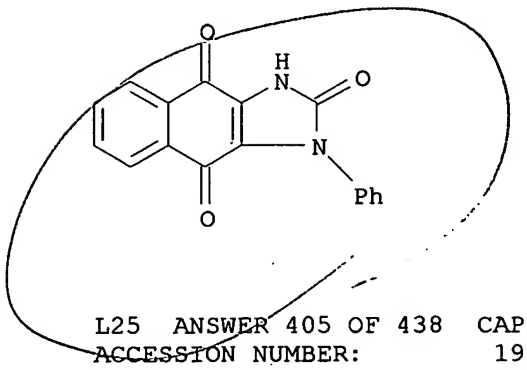
L25 ANSWER 404 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1967:403030 CAPLUS
DOCUMENT NUMBER: 67:3030
TITLE: Naphth[2,3-d]imidazoline-2,4,9-triones
AUTHOR(S): Truitt, Price; Witkowski, J. T.
CORPORATE SOURCE: N. Texas State Univ., Denton, TX, USA
SOURCE: Canadian Journal of Chemistry (1967), 45(9), 997-9
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.

AB 1-Substituted naphth[2,3-d]-imidazoline-2,4,9-triones (I) were prepared by base-catalyzed cyclization of 1-benzoyl-3-(3-substituted-1,4-dihydro-1,4-dioxo-2-naphthyl)ureas and of 2-(ethoxycarbonylamino)-3-substituted-1,4-naphthoquinones.

IT **16223-62-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 16223-62-4 CAPLUS

CN 1H-Naphth[2,3-d]imidazole-2,4,9(3H)-trione, 1-phenyl- (8CI, 9CI) (CA INDEX NAME)



closest so far

L25 ANSWER 405 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1966:19271 CAPLUS

DOCUMENT NUMBER: 64:19271

ORIGINAL REFERENCE NO.: 64:3519e-h,3520a-f

TITLE: Potential antimycobacterial agents. XVII. Synthesis of some cyclic analogs of thiocarbanilides

AUTHOR(S): Mathur, K. B.; Bhaduri, A. P.; Iyer, R. N.; Khanna, N. M.; Dhar, M. L.

CORPORATE SOURCE: Central Drug Res. Inst., Lucknow

SOURCE: Indian Journal of Chemistry (1965), 3(9), 397-401
CODEN: IJOCAP; ISSN: 0019-5103

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB cf. CA 57, 11183a. Several 6-alkoxy-2-(p-alkoxyphenylamino)benzothiazoles, 6-alkoxy-1-(p-alkoxyphenyl)-2-mercaptobenzimidazoles (I), 6-alkyloxybenzimodazole-2-thioglycolic acids, esters and substituted amides and hydrazides (II, R1 = OH, OEt, and NHNH2 resp.) and α,ω-bis(6-alkoxybenzimidazol-2-yl)alkane, dithio ethers (III) were synthesized as structural analogs of the biologically active diarylthioureas in the hope that such compds. may be absorbed more efficiently from the gastrointestinal tract. Thus, a solution of 1.6 g. Br in 50 ml. CHCl3 was added dropwise with stirring to a suspension of 3.16 g. 4,4'-diethoxythiocarbanilide (Hugerschoff, Chemical Ber. 32, 2246(1899)). The reaction mixture was left 3 hrs. at room temperature, washed successively with H2O, 5% NaHSO3, 10% NaOH, and H2O. The organic layer was dried (Na2SO4) and the solvent removed in vacuo to yield 2.2 g. 6-ethoxy-2-(p-ethoxyphenylamino)benzothiazole, m. 152° (C6H6) (after chromatography over Al2O3 using C6H6 as eluant). Similarly, 4,4'-diisoamyloxythiocarbanilide yielded 6-isoamyloxy-2-(p-isoamyloxyphenylamino)benzothiazole, m. 105° (C6H6-petr. ether). I were prepared by reducing the appropriate 4',5-bis(alkyloxy)-2-nitrodiphenylamines (IV) with H and Raney Ni. IV required for the work were prepared as follows: A mixture of 4 g. phenetidine, 4 g. 4-ethoxy-2-nitrochlorobenzene, 6 g. fused NaOAc, and 4 ml. HCONMe2 was heated 10 hrs. at 190-200°. The reaction mixture was dissolved in min. volume of EtOH, acidified (1:1 HCl), diluted with H2O, and repeatedly extracted with C6H6. The C6H6 extract was dried (Na2SO4), solvent removed in vacuo, and the residue extracted with hot petr. ether. Cooling of the petr.

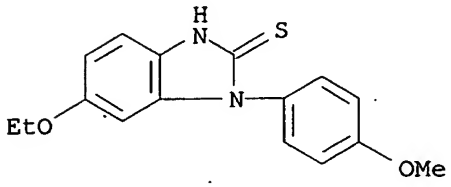
ether extract yielded 4',5-diethoxy-2-nitrodiphenylamine IV (R = R1 = Me), m. 107° (hexane) (after chromatography over Al2O3 using C6H6-hexane (20:80) for elution). The following IV were similarly prepared (R, R1, and m.p. given): Me, Me, 107° (EtOH); Me, Et, 138° (EtOH); Me, iso-C5H11, 71° (hexane); Et, Me, 113° (hexane); Bu, Et, 69° (hexane); iso-C5H11, iso-C5H11 (IVa), 66° (hexane). In the case of IVa, a semi-solid was obtained after chromatography. When heated at 3 mm. a small quantity of orange-red oil distilled at 205-50°. Rechromatography of the residue using C6H6-hexane (20:80) as eluant yielded pure IVa. IV (R = R1 = Et), (1.5 g.) in 40 ml. EtOH was hydrogenated at 30 lb./in.2 in presence of Raney Ni. After 30 min. of further agitation, the reaction mixture, containing 2-amino-4',5-diethoxydiphenylamine, was immediately filtered into a solution of 0.67 g. K ethyl xanthate in 15 ml. EtOH. The mixture was refluxed 10 hrs., EtOH removed in vacuo, residue acidified (10% HOAc), solid dissolved in C6H6, and the solution chromatographed over Al2O3 using initially C6H6 for removing impurities followed by EtOH to yield 0.85 g. 6-ethoxy-1-(p-ethoxyphenyl)-2-mercaptobenzimidazole (I, R = R1 = Et), m. 199° (EtOH). Following I were similarly prepared (R, R1, and m.p. given): Me, Me, 207° (C6H6); Me, Et, 196° (C6H6); Me, iso-C5H11, 186° (EtOH); Et, Et, 200° (EtOH); Bu, Et, 173° (EtOH); iso-C5H11, iso-C5H11, 154° (EtOH). Reaction of 6-alkoxy-2-mercaptobenzimidazoles with monochloroethyl acetate in the presence of NaOEt (6 hrs. heating on water bath) yielded 6-alkyloxybenzimidazole-2-thioglycolic esters (II, R1 = Et) (ν 1725 cm.-1), which on hydrolysis with 20% aqueous NaOH (1 hr. heating on water bath) gave the corresponding acids (II, R1 = OH) (ν 1705 cm.-1) and on treatment with N2H4H2O (heating 3 hrs., water bath) yielded the required hydrazide (II, R1 = NHNH2). Attempts to condense the ester with primary or secondary amines failed to yield the amides. The conversion of the acid (II, R = OH) into its acid chloride at low temperature followed by reaction of the latter with amine yielded the desired product in poor yields. The same compds. could, however, be prepared in good yields by the reaction of the acids with the appropriate amine in the presence of dicyclohexylcarbodiimide. Following II were prepared: (R, R1, and m.p. given): Me, OEt, 82-3°; Me, OH, 197-8°; Me, NHNH2, 131-2°; Et, OEt, 108-9°; Et, OH, 167-8°; Et, NHNH2, 116-17°; Et, NH-Ph, 150-1°; Et, piperidyl, 69-70°; Et, NHCH2C6H4OMe-p, 142-3°; Et, NHC6H4OEt-p, 182-3°; Et, NHC6H3F2-2,4, 154-5°; iso-C5H11, OEt, 90-1°; iso-C5H11, OH, 178°. Pentamethylene diiodide (0.8 g.) was added to a warm solution of 1.2 g. 6-iso-amyloxy-2-mercaptobenzimidazole and NaOEt (prepared from 0.12 g. Na and 50 ml. absolute EtOH). The mixture was refluxed 8 hrs., cooled, diluted with H2O, extracted with CHCl3, extract dried, and solvent removed to yield 0.7 g. III. Following III were prepared by using different iodides (R, n, and m.p. given): iso-C5H11, 10, 92-3°; iso-C5H11, 9, -- (hygroscopic, isolated as dihydrochloride); iso-C5H11, 5, 55-6°; Me, 10, 43-4°; Et, 10, 42-3°. A solution of 10 g. 4,4'-diethoxydiphenylthiourea in a mixture of dry CHCl3 and dry C6H6 (3:1, 350 ml.) and 9 g. MeI was left 100 hrs. at room temperature to yield 10 g. 3-methyl-4,4'-diethoxydiphenyl iso-thiuronium hydriodide, m. 167-8° (CHCl3-petr. ether), ν 1600 cm.-1 Use of 1.5 g. 4,4'-dibutoxydiphenylthiourea in the above experiment yielded 1 g. 3-methyl-4,4'-dibutoxydiphenylisothiuronium hydriodide, m. 131-2°. None of the compds. were found to possess significant antimycobacterial activity.

IT **4793-94-6**, 2-Benzimidazolinethione, 6-ethoxy-1-(p-methoxyphenyl)- **4813-86-9**, 2-Benzimidazolinethione, 6-(isopentyloxy)-1-[p-(isopentyloxy)phenyl]- **4847-54-5**, 2-Benzimidazolinethione, 6-ethoxy-1-(p-ethoxyphenyl)- **4847-55-6**, 2-Benzimidazolinethione, 1-[p-(isopentyloxy)phenyl]-6-methoxy- **4983-84-0**, 2-Benzimidazolinethione, 6-methoxy-1-(p-methoxyphenyl)- **4983-86-2**, 2-Benzimidazolinethione, 1-(p-ethoxyphenyl)-6-methoxy- **4983-87-3**

, 2-Benzimidazolinethione, 6-butoxy-1-(p-ethoxyphenyl)-
(preparation of)

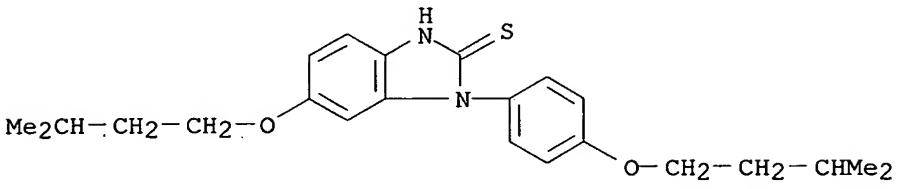
RN 4793-94-6 CAPLUS

CN 2-Benzimidazolinethione, 6-ethoxy-1-(p-methoxyphenyl)- (7CI, 8CI) (CA INDEX NAME)



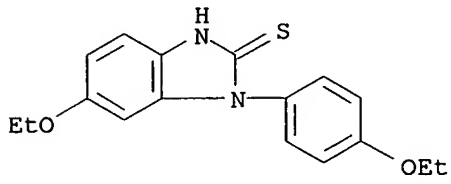
RN 4813-86-9 CAPLUS

CN 2-Benzimidazolinethione, 6-(isopentyloxy)-1-[p-(isopentyloxy)phenyl]- (7CI, 8CI) (CA INDEX NAME)



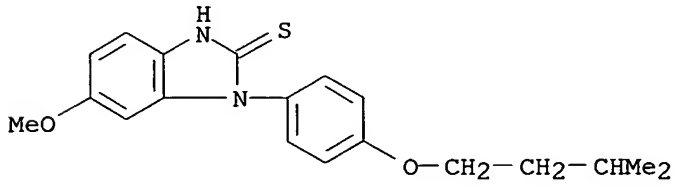
RN 4847-54-5 CAPLUS

CN 2-Benzimidazolinethione, 6-ethoxy-1-(p-ethoxyphenyl)- (7CI, 8CI) (CA INDEX NAME)



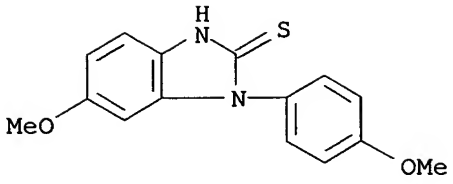
RN 4847-55-6 CAPLUS

CN 2-Benzimidazolinethione, 1-[p-(isopentyloxy)phenyl]-6-methoxy- (7CI, 8CI) (CA INDEX NAME)

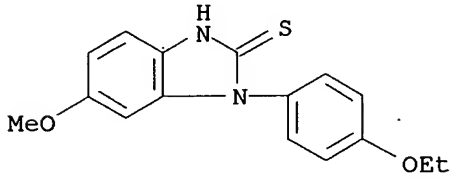


RN 4983-84-0 CAPLUS

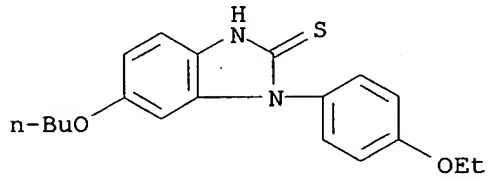
CN 2-Benzimidazolinethione, 6-methoxy-1-(p-methoxyphenyl)- (7CI, 8CI) (CA INDEX NAME)



RN 4983-86-2 CAPLUS
CN 2-Benzimidazolinethione, 1-(p-ethoxyphenyl)-6-methoxy- (7CI, 8CI) (CA INDEX NAME)



RN 4983-87-3 CAPLUS
CN 2-Benzimidazolinethione, 6-butoxy-1-(p-ethoxyphenyl)- (7CI, 8CI) (CA INDEX NAME)



L25 ANSWER 406 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1966:11511 CAPLUS
DOCUMENT NUMBER: 64:11511
ORIGINAL REFERENCE NO.: 64:2093b-g
TITLE: Benzimidazolones
PATENT ASSIGNEE(S): Dr. A. Wander A.-G.
SOURCE: 19 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 659364		19650805	BE	
NL 6501434			NL	
PRIORITY APPLN. INFO.:			CH	19640205

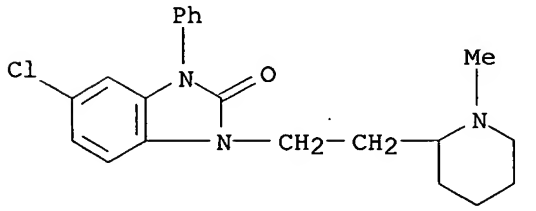
GI For diagram(s), see printed CA Issue.
AB The title compds. (I) were prepared Thus, 7.5 g. 1; phenylbenzimidazolone in 50 ml. absolute dioxane was refluxed with 1.68 g. NaNH2 for 1 hr. Then, 5.4 g. β-dimethylaminoethyl chloride in 30 ml. C6H6 was added and the mixture refluxed 16 hrs. to yield 88% 1 phenyl-3-β-dimethylaminoethylbenzimidazolone (II), m. 116-17° (acetone-ligroine). Alternately, heating 12.3 g. N-phenyl-N1-(β-dimethylamino)ethyl-o-phenylenediamine with 4 g. urea at 200° for 15 hrs. yielded 8.4 g. II. Similarly, 6.1 g. 1-phenyl-6-chlorobenzimidazolone (III) was boiled with 1 g. K in 40 ml.

tert-BuOH for 10 min. After the mixture was evaporated to dryness in vacuo, the K compound was mixed with 40 ml. dimethylformamide and heated with 4.8 g. freshly distilled 1-methyl-3-chloromethylpiperazine at 50° for 18 hrs. to yield 2.7 g. 1-phenyl-3-(1-methyl-3-piperidyl)methyl-6-chlorobenzimidazolone, m. 112-14° (ether-ligroine), and 2.7 g. unreacted III. In like manner, 7.3 g. III in 40 ml. absolute dioxane was refluxed with 1.2 g. K in 30 ml. tert-BuOH for 1 hr. After addition of 5.7 g. trimethylene chloro bromide, the mixture was refluxed an addition 7 hrs. The reaction mixture was concentrated and the residue was distributed between H2O and ether. The ether solution was washed with H2O and evaporated to dryness. The residue (6.4 g.) was heated with 5 g. Me2NH in 20 ml. dioxane in a sealed tube for 18 hrs. to yield 4.9 g. 1-phenyl-3-γ-dimethylaminopropyl-6-chlorobenzimidazolone (IV), b0.03 163°; IV.HCl m. 180-2°. Alternately, 6.3 g. 1-phenyl-3-γ-aminopropyl-6-chlorobenzimidazolone was heated with 10 ml. 90% HCO2H and 5 ml. 35% CH2O at 100° for 15 hrs. After addition of 2 ml. 38% HCl the mixture was evaporated to dryness to yield 6.1 g. IV.HCl, m. 180-2°. When 8.7 g. 1-p-aminophenyl-3-γ-(pyrrolidin-1-yl)propylbenzimidazolone was diazotized and treated with CuCl2 in the usual manner 5.6 g. 1-p-chlorophenyl-3-γ-(pyrrolidin-1-yl)propylbenzimidazolone, m. 54-6° (ligroine), was obtained. Other derivs. prepared are (R2R3NQR1, R4, R5, and physical consts. given): (CH2)3NEt2, H, H, HCl salt m. 153-5°; (CH2)2NMe2, 5-Cl, H, m. 127-8°; (CH2)3NMe2, 5-Cl, H, m. 104-5°, (CH2)2NMe2, 6-Cl, H, m. 111-12°; 2-(1-methyl-2-piperidyl)ethyl, 6-Cl, H, b. 210°/0.05 mm.; (CH2)2NMe2, H, p-Cl, m. 114-15°; (CH2)3NMe2, H, p-Cl, b. 176-7°/0.01 mm., HCl salt m. 232-6°; (CH2)3NMe2, 5-Me, H, m. 75-6°; (CH2)3NEt2, 6-Cl, H, HCl salt m. 184-5°; 3-pyrrolidinopropyl, 6-Cl, H, m. 75-6°; 3-piperidinopropyl, 6-Cl, H, m. 97-9°; (CH2)3NHMe, 6-Cl, H, m. 88-90°; (CH2)3NEt2, H, p-Cl, m. 52-4°; (CH2)3NMe2, 6-Cl, p-Cl, m. 102-3°; 3-piperidinopropyl, H, p-Cl, m. 102-3°; 2-(1-methyl-2-piperidyl)ethyl, H, p-Cl, m. 127-9°; 2-(1-methyl-3-piperidyl)ethyl, H, p-Cl, HCl salt m. 217° (decomposition); (CH2)3NEt2, H, p-Me, m. 51-2°; 3-pyrrolidinomethyl, H, p-Me, m. 85-7°; (CH2)3NEt2, H, p-Br, HCl salt m. 198-9°; (CH2)3NEt2, H, p-F, m. 39.5-41°, (CH2)3NMe2, H, p-F, HCl salt m. 200-2°; (CH2)3NEt2, H, o-Cl, b. 186°/0.05 mm.; 3-pyrrolidinopropyl, H, o-Cl, HCl salt m. 174-8°; (CH2)3NEt2, H, m-Cl, m. 48-52°; 3-pyrrolidinopropyl, H, m-Cl, m. 75-7°. The compds. are useful as antidepressives and anticonvulsants.

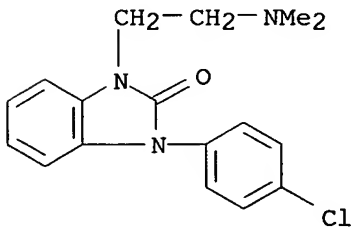
IT **4750-40-7**, 2-Benzimidazolinone, 5-chloro-1-[2-(1-methyl-2-piperidyl)ethyl]-3-phenyl- **4750-41-8**, 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-[2-(dimethylamino)ethyl]- **4750-42-9**, 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-[3-(dimethylamino)propyl]- **4750-43-0**, 2-Benzimidazolinone, 3-[3-(dimethylamino)propyl]-5-methyl-1-phenyl- **4750-45-2**, 2-Benzimidazolinone, 5-chloro-3-phenyl-1-[3-(1-pyrrolidinyl)propyl]- **4750-46-3**, 2-Benzimidazolinone, 5-chloro-3-phenyl-1-(3-piperidinopropyl)- **4750-47-4**, 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-[3-(diethylamino)propyl]- **4750-48-5**, 2-Benzimidazolinone, 5-chloro-3-(p-chlorophenyl)-1-[3-(dimethylamino)propyl]- **4750-49-6**, 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-[2-(1-methyl-2-piperidyl)ethyl]- **4750-50-9**, 2-Benzimidazolinone, 1-[3-(diethylamino)propyl]-3-p-tolyl- **4750-51-0**, 2-Benzimidazolinone, 1-[3-(1-pyrrolidinyl)propyl]-3-p-tolyl- **4750-54-3**, 2-Benzimidazolinone, 1-(m-chlorophenyl)-3-[3-(diethylamino)propyl]- **4750-55-4**, 2-Benzimidazolinone, 1-(m-chlorophenyl)-3-[3-(1-pyrrolidinyl)propyl]- **4755-58-2**, 2-Benzimidazolinone, 1-[2-(dimethylamino)ethyl]-3-phenyl- **4755-59-3**, 2-Benzimidazolinone, 5-chloro-1-[3-

(dimethylamino)propyl]-3-phenyl- **4755-60-6**, 2-Benzimidazolinone, 5-chloro-3-[3-(dimethylamino)propyl]-1-phenyl- **4755-61-7**, 2-Benzimidazolinone, 5-chloro-1-[2-(dimethylamino)ethyl]-3-phenyl- **4794-92-7**, 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-(3-piperidinopropyl)- **4794-93-8**, 2-Benzimidazolinone, 1-[3-(diethylamino)propyl]-3-(p-fluorophenyl)- **4795-94-2**, 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-[3-(1-pyrrolidinyl)propyl]- **4819-25-4**, 2-Benzimidazolinone, 1-(o-chlorophenyl)-3-[3-(diethylamino)propyl]- **4870-78-4**, 2-Benzimidazolinone, 5-chloro-1-[(1-methyl-3-piperidyl)methyl]-3-phenyl- **4870-79-5**, 2-Benzimidazolinone, 1-[3-(diethylamino)propyl]-3-phenyl-, hydrochloride **4891-91-2**, 2-Benzimidazolinone, 5-chloro-3-[2-(dimethylamino)ethyl]-1-phenyl- **5605-58-3**, 2-Benzimidazolinone, 5-chloro-1-[3-(methylamino)propyl]-3-phenyl- **21731-63-5**, 2-Benzimidazolinone, 5-chloro-1-[3-(dimethylamino)propyl]-3-phenyl-, hydrochloride **21731-70-4**, 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-[3-(dimethylamino)propyl]-, hydrochloride **21741-79-7**, 2-Benzimidazolinone, 5-chloro-1-[3-(diethylamino)propyl]-3-phenyl-, hydrochloride **21741-86-6**, 2-Benzimidazolinone, 1-(p-bromophenyl)-3-[3-(diethylamino)propyl]-, hydrochloride **21741-88-8**, 2-Benzimidazolinone, 1-[3-(dimethylamino)propyl]-3-(p-fluorophenyl)-, hydrochloride **21741-90-2**, 2-Benzimidazolinone, 1-(o-chlorophenyl)-3-[3-(1-pyrrolidinyl)propyl]-, hydrochloride **21808-04-8**, 2-Benzimidazolinone, 1-p-chlorophenyl)-3-[(1-methyl-3-piperidyl)methyl]-, hydrochloride
(preparation of)

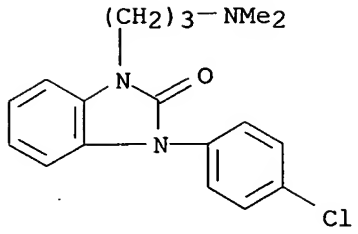
RN 4750-40-7 CAPLUS
CN 2-Benzimidazolinone, 5-chloro-1-[2-(1-methyl-2-piperidyl)ethyl]-3-phenyl- (7CI, 8CI) (CA INDEX NAME)



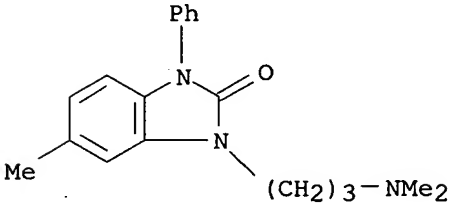
RN 4750-41-8 CAPLUS
CN 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-[2-(dimethylamino)ethyl]- (7CI, 8CI) (CA INDEX NAME)



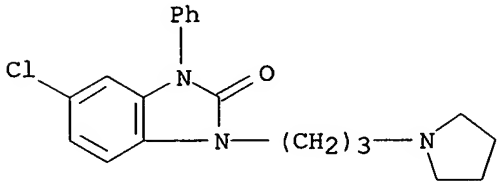
RN 4750-42-9 CAPLUS
CN 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-[3-(dimethylamino)propyl]- (8CI) (CA INDEX NAME)



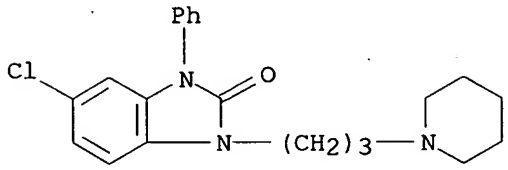
RN 4750-43-0 CAPLUS
CN 2-Benzimidazolinone, 3-[3-(dimethylamino)propyl]-5-methyl-1-phenyl- (7CI, 8CI) (CA INDEX NAME)



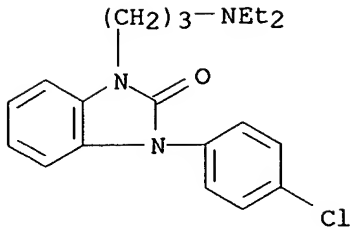
RN 4750-45-2 CAPLUS
CN 2-Benzimidazolinone, 5-chloro-3-phenyl-1-[3-(1-pyrrolidinyl)propyl]- (7CI, 8CI) (CA INDEX NAME)



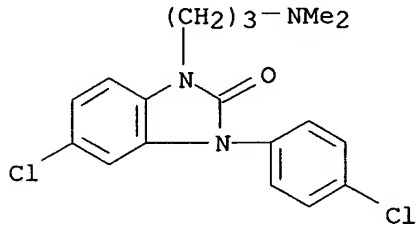
RN 4750-46-3 CAPLUS
CN 2-Benzimidazolinone, 5-chloro-3-phenyl-1-(3-piperidinopropyl)- (7CI, 8CI) (CA INDEX NAME)



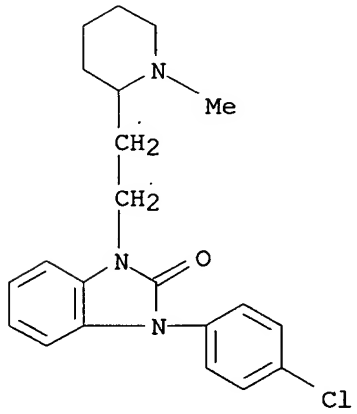
RN 4750-47-4 CAPLUS
CN 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-[3-(diethylamino)propyl]- (7CI, 8CI) (CA INDEX NAME)



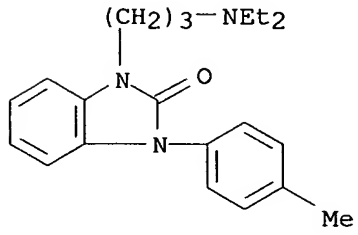
RN 4750-48-5 CAPLUS
CN 2-Benzimidazolinone, 5-chloro-3-(p-chlorophenyl)-1-[3-(dimethylamino)propyl]- (7CI, 8CI) (CA INDEX NAME)



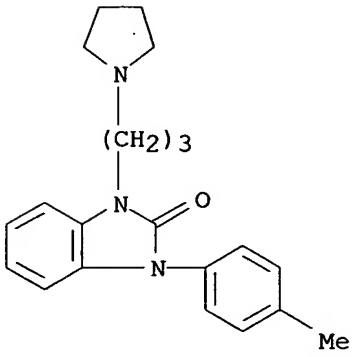
RN 4750-49-6 CAPLUS
CN 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-[2-(1-methyl-2-piperidyl)ethyl]- (7CI, 8CI) (CA INDEX NAME)



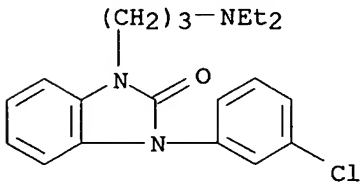
RN 4750-50-9 CAPLUS
CN 2-Benzimidazolinone, 1-[3-(diethylamino)propyl]-3-p-tolyl- (7CI, 8CI) (CA INDEX NAME)



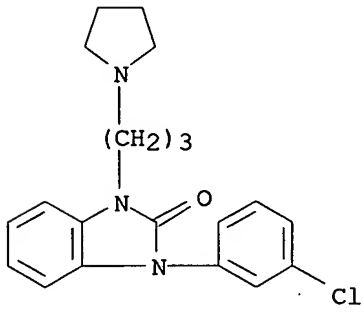
RN 4750-51-0 CAPLUS
CN 2-Benzimidazolinone, 1-[3-(1-pyrrolidinyl)propyl]-3-p-tolyl- (7CI, 8CI) (CA INDEX NAME)



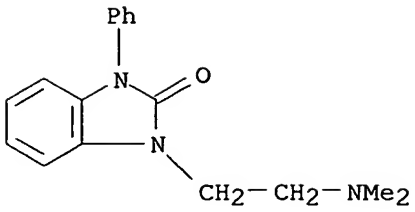
RN 4750-54-3 CAPLUS
CN 2-Benzimidazolinone, 1-(m-chlorophenyl)-3-[3-(diethylamino)propyl]- (7CI, 8CI) (CA INDEX NAME)



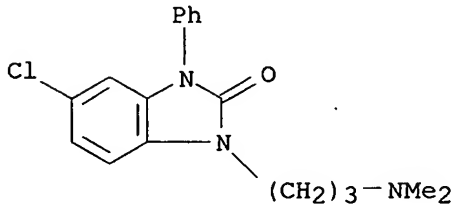
RN 4750-55-4 CAPLUS
CN 2-Benzimidazolinone, 1-(m-chlorophenyl)-3-[3-(1-pyrrolidinyl)propyl]- (7CI, 8CI) (CA INDEX NAME)



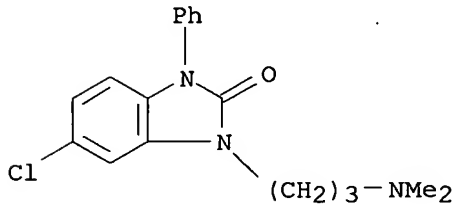
RN 4755-58-2 CAPLUS
CN 2-Benzimidazolinone, 1-[2-(dimethylamino)ethyl]-3-phenyl- (7CI, 8CI) (CA INDEX NAME)



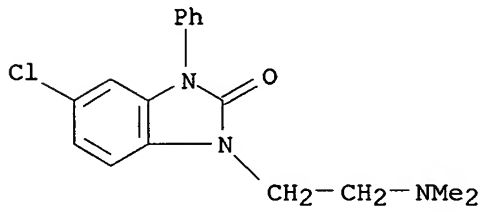
RN 4755-59-3 CAPLUS
CN 2H-Benzimidazol-2-one, 5-chloro-1-[3-(dimethylamino)propyl]-1,3-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



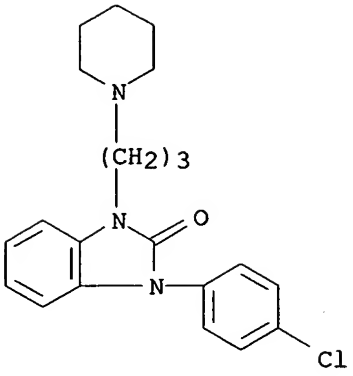
RN 4755-60-6 CAPLUS
CN 2-Benzimidazolinone, 5-chloro-3-[3-(dimethylamino)propyl]-1-phenyl- (8CI) (CA INDEX NAME)



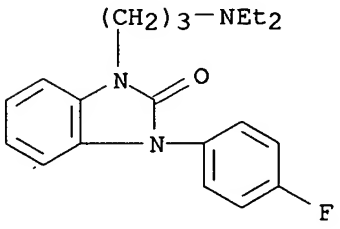
RN 4755-61-7 CAPLUS
CN 2-Benzimidazolinone, 5-chloro-1-[2-(dimethylamino)ethyl]-3-phenyl- (7CI, 8CI) (CA INDEX NAME)



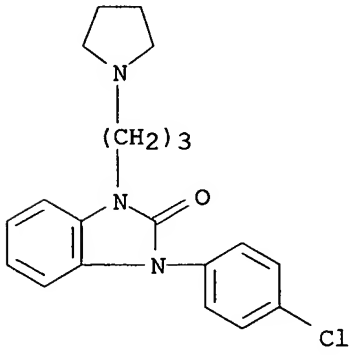
RN 4794-92-7 CAPLUS
CN 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-(3-piperidinopropyl)- (7CI, 8CI) (CA INDEX NAME)



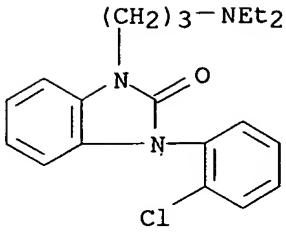
RN 4794-93-8 CAPLUS
CN 2-Benzimidazolinone, 1-[3-(diethylamino)propyl]-3-(p-fluorophenyl)- (7CI, 8CI) (CA INDEX NAME)



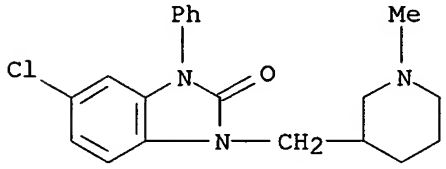
RN 4795-94-2 CAPLUS
CN 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-[3-(1-pyrrolidinyl)propyl]- (7CI, 8CI) (CA INDEX NAME)



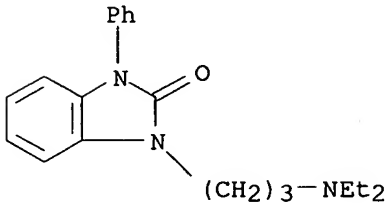
RN 4819-25-4 CAPLUS
CN 2-Benzimidazolinone, 1-(o-chlorophenyl)-3-[3-(diethylamino)propyl]- (7CI, 8CI) (CA INDEX NAME)



RN 4870-78-4 CAPLUS
CN 2-Benzimidazolinone, 5-chloro-1-[(1-methyl-3-piperidyl)methyl]-3-phenyl- (7CI, 8CI) (CA INDEX NAME)

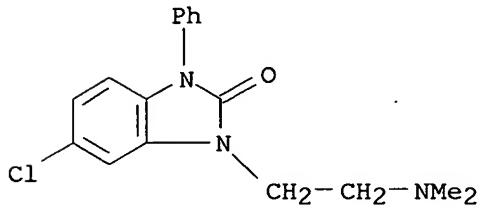


RN 4870-79-5 CAPLUS
CN 2-Benzimidazolinone, 1-[3-(diethylamino)propyl]-3-phenyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)

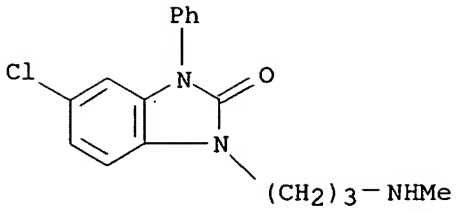


● HCl

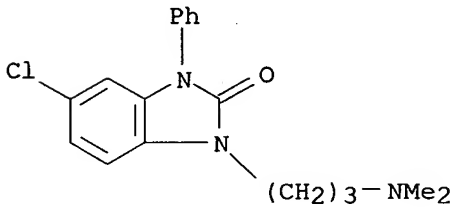
RN 4891-91-2 CAPLUS
CN 2-Benzimidazolinone, 5-chloro-3-[2-(dimethylamino)ethyl]-1-phenyl- (7CI, 8CI) (CA INDEX NAME)



RN 5605-58-3 CAPLUS
CN 2-Benzimidazolinone, 5-chloro-1-[3-(methylamino)propyl]-3-phenyl- (7CI, 8CI) (CA INDEX NAME)

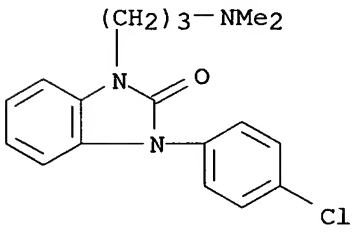


RN 21731-63-5 CAPLUS
CN 2-Benzimidazolinone, 5-chloro-1-[3-(dimethylamino)propyl]-3-phenyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



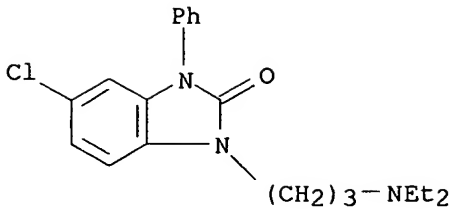
●x HCl

RN 21731-70-4 CAPLUS
CN 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-[3-(dimethylamino)propyl]-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



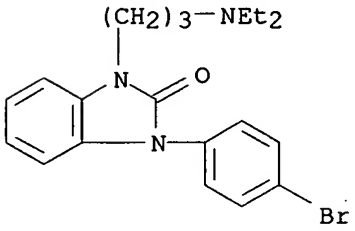
●x HCl

RN 21741-79-7 CAPLUS
CN 2-Benzimidazolinone, 5-chloro-1-[3-(diethylamino)propyl]-3-phenyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



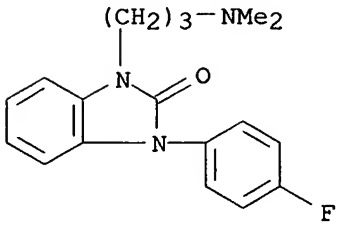
●x HCl

RN 21741-86-6 CAPLUS
CN 2-Benzimidazolinone, 1-(p-bromophenyl)-3-[3-(diethylamino)propyl]-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



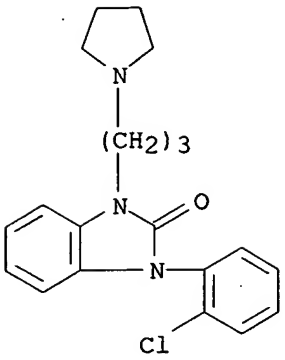
●x HCl

RN 21741-88-8 CAPLUS
CN 2-Benzimidazolinone, 1-[3-(dimethylamino)propyl]-3-(p-fluorophenyl)-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



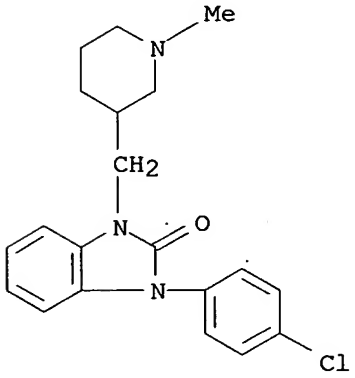
●x HCl

RN 21741-90-2 CAPLUS
CN 2-Benzimidazolinone, 1-(o-chlorophenyl)-3-[3-(1-pyrrolidinyl)propyl]-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



●x HCl

RN 21808-04-8 CAPLUS
CN 2-Benzimidazolinone, 1-(p-chlorophenyl)-3-[(1-methyl-3-piperidyl)methyl]-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



●x HCl

L25 ANSWER 407 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1965:460905 CAPLUS
DOCUMENT NUMBER: 63:60905
ORIGINAL REFERENCE NO.: 63:11075g-h
TITLE: Floatability of antlerite from Udokansk deposit
AUTHOR(S): Demidovich, G. I.; Kislyakov, L. D.
SOURCE: Tsvetnye Metally (Moscow, Russian Federation) (1965), 38(4), 21
CODEN: TVMTAX; ISSN: 0372-2929
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

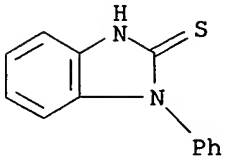
AB The floatability of antlerite, Cu[SO4][OH]4, was examined Of the Cu content, 5-7% was soluble in aqueous solution of aero-float, indicating a possible Cu loss in flotation. Best flotation conditions were weakly alkaline medium (16 g. free CaO/cu. m. liquid), high xanthate consumption (≤93 g. moles/ton without sulfidization), and grinding to 100% -0.104 mm. In comparison with butylxanthate; the use of the new collector dicyclohexyldithiocarbamate increased antlerite extraction markedly. Even more

effective was 1-phenyl-2-mercaptobenzimidazole, which gave complete extraction of antlerite at a consumption of 0.24 g. mole/ton without sulfidization. Without sulfidization, antlerite was floated more actively than was malachite. Flotation of malachite and antlerite with butylxanthate and sulfidization gave identical results.

IT **4493-32-7**, 2-Benzimidazolethiol, 1-phenyl-
(antlerite flotation by)

RN 4493-32-7 CAPLUS

CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



L25 ANSWER 408 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1965:429886 CAPLUS

DOCUMENT NUMBER: 63:29886

ORIGINAL REFERENCE NO.: 63:5279h,5280a-b

TITLE: Physicochemical and flotation properties of substituted benzimidazolethiones

AUTHOR(S): Kakovskii, I. A.; Tyurenkova, G. N.

SOURCE: Izvestiya Vysshikh Uchebnykh Zavedenii, Tsvetnaya Metallurgiya (1965), 8(1), 21-7
CODEN: IVUTAK; ISSN: 0021-3438

DOCUMENT TYPE: Journal

LANGUAGE: Russian

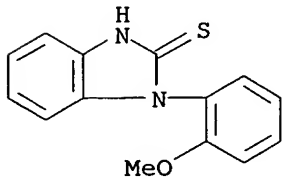
GI For diagram(s), see printed CA Issue.

AB A series of active anionic collectors for the oxidized minerals of Pb and Cu was developed with the structure I, where R is a C4+ alkyl, aryl, or aralkyl. These reagents are very powerful collectors and their characteristics for this use are described (CA 57, 14769i; 58, 280h).

IT **3387-18-6**, 2-Benzimidazolinethione, 1-(o-methoxyphenyl)-
3387-19-7, 2-Benzimidazolinethione, 1-(p-chlorophenyl)-
4493-32-7, 2-Benzimidazolinethione, 1-phenyl- **26495-07-8**, 2-Benzimidazolinethione, 1-(p-methoxyphenyl)-
(as flotation agent for Cu-Pb oxidized ores)

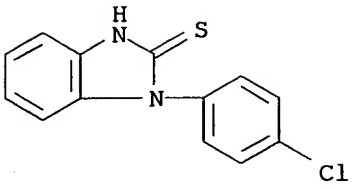
RN 3387-18-6 CAPLUS

CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)

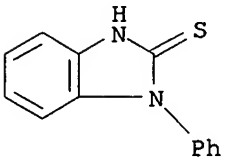


RN 3387-19-7 CAPLUS

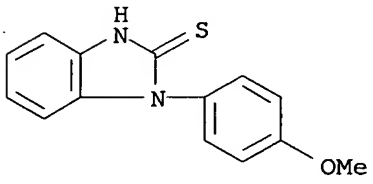
CN 2H-Benzimidazole-2-thione, 1-(4-chlorophenyl)-1,3-dihydro- (9CI) (CA INDEX NAME)



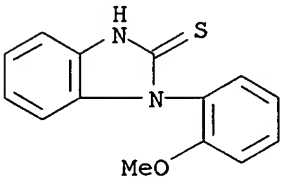
RN 4493-32-7 CAPLUS
CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



RN 26495-07-8 CAPLUS
CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



IT **3387-18-6**, 2-Benzimidazolinethione, 1-(o-methoxyphenyl)-
(preparation of)
RN 3387-18-6 CAPLUS
CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



L25 ANSWER 409 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1965:9119 CAPLUS
DOCUMENT NUMBER: 62:9119
ORIGINAL REFERENCE NO.: 62:1660h,1661a-e
TITLE: Diuretics. I. 8-Sulfamoyltheophylline and 7-substituted derivatives
AUTHOR(S): Dolman, H.; van der Goot, J.; Mos, G. H.; Moed, H. D.
CORPORATE SOURCE: N. V. Philips-Duphar Res. Labs., Weesp, Neth.
SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1964), 83(9/10), 1215-29
CODEN: RTCPA3; ISSN: 0165-0513
DOCUMENT TYPE: Journal

LANGUAGE: English

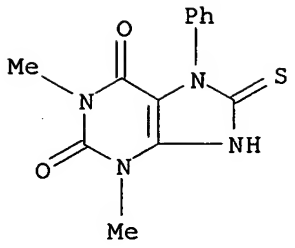
GI For diagram(s), see printed CA Issue.

AB I (R1 = Cl) (Ia, R = PhCH2), m. 152-4° (alc.-C6H6), was prepared in 77% yield by refluxing 8-chlorotheophylline (II), NaOH, and PhCH2Cl in aqueous alc. Excellent yields were also obtained when 1 part Na salt of II and 1 part of the appropriate halide was refluxed in HCONMe2 (DMF). Thus prepared were the following Ia (R, m.p., and % yield given): Me(CH2)5, 75-80° (alc.-C6H6), 78; cyclohexylmethyl, 152-4°, 77; Ph(CH2)2, 152-4° (alc.), 36; Ph(CH2)3, 108-9° (aqueous Me2CO), 54; PhCH2OCH2CH2, 100-2° (alc.), 70. A mixture of 57 g. Na theophyllinate, 45 g. p-ClC6H4NO2, and 300 ml. DMF was refluxed 20 hrs. to yield 47 g. 7-(p-nitrophenyl)theophylline (III), m. 325-7° (HOAc-DMF). III (88 g.) was treated with excess Cl to give 71 g. the 8-chloro derivative (IV), m. 242-2.5° (alc.-C6H6). To a suspension of 5 g. IV in 100 ml. alc., a solution of 29 g. FeSO4.7H2O in 400 ml. H2O was added, and the mixture refluxed under N, treated with 17 ml. 25% aqueous NH3 and 50 ml. H2O, and refluxed 1.5 hrs. to yield 4.2 g. the 7-(p-aminophenyl) analog (V), m. 255-7° (alc.-C6H6). A solution of 22.5 g. V in 110 ml. 30% H2PO3, 30 ml. HOAc, and 80 ml. H2O cooled to 0° was treated with 5.39 g. NaNO2 in 25 ml. H2O in the presence of a little Et2O and kept overnight at 10° to give 20 g. Ia (R = Ph) (VI), m. 259.5-60° (alc.-C6H6). 7-(p-Aminophenyl)theophylline (VII), m. 278-9°, was obtained in 45% yield by refluxing III with Na2S and NH3 in alc., and in 95% yield when III and SnCl2 were refluxed in N HCl. 7-Phenyltheophylline m. 193-4.5° (alc.). A solution of 28 g. KOH in 650 ml. H2O was saturated with H2S and refluxed 3 hrs. with 52 g. VI and 50 ml. BuOCH2CH2OH to give 46 g. I (R1 = SH) (VIII, R = PhCH2), m. 290-3°. Similarly prepared were the following VIII (R, m.p., and % yield given): Me(CH2)5, 210-14° (alc.), 45; cyclohexylmethyl, 291-4°, 78; Ph(CH2)2, 290-2°, 86; Ph(CH2)3, 233-3.5°, 84; PhCH2OCH2CH2, 174-7°, 82; Ph, m. 248-52°, 78. During 1 hr. 16 ml. Br was added to a suspension of 0.1 mole VIII in 600 ml. N HCl containing a crystal of FeCl3 and some KBr, and the mixture stirred 15 min. at 0-5°. The crude sulfobromide was dissolved in 600 ml. ice-cold 25% aqueous NH3, kept 45 min. (warmed if necessary), excess NH3 removed in vacuo, and HCl added to precipitate the following I (R1 = SO2NH2) (IX) (R, m.p., and % yield given): cyclohexylmethyl, 250-2°, 33; PhCH2, 199-201°, 63; Ph(CH2)2, 224-6°, 50; Ph, 281° (decomposition), 16. Br (16 ml.) added (ice-bath) to a suspension of 0.1 mole VIII in a mixture of 450 ml. 0.25N HCl and 350 ml. CHCl3, FeSO3.7H2O added to remove excess Br, and the CHCl3 layer treated with gaseous NH3 afforded IX (R, m.p., and % yield given): Me(CH2)5, 165-5.5°, 32; Ph(CH2)3, 178-80°, 11; PhCH2OCH2CH2, 181-3°, 16. IX (R = H), m. 299° (decomposition), was prepared in 0.9-g. yield when 3.2 g. IX (R = Ph) was refluxed 20 min. in a mixture of 6 ml. HOAc and 30 ml. 45% HBr. 8-Mercaptocaffeine (5 g.) in 70 ml. 25% aqueous NH3 was treated dropwise with a solution of 15 g. K3Fe(CN)6 in 50 ml. H2O at -5°. After the formation of a yellow precipitate, 40 ml. 5% aqueous KMnO4 was added to give 2.5 g. 8-sulfamoylcaffeine, decomposing at 245-7°. IX (R = H) appeared to have no diuretic properties, but IX (R = PhCH2) exhibited an appreciable diuretic activity, while lacking other pharmacol. properties of theophylline. This compound inhibited carbonic anhydrase.

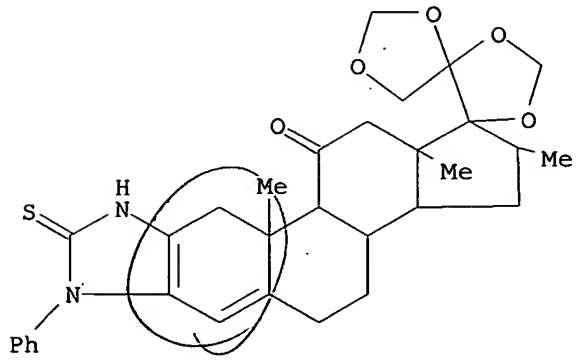
IT **963-43-9**, Uric acid, 1,3-dimethyl-7-phenyl-8-thio-
(preparation of)

RN 963-43-9 CAPLUS

CN Uric acid, 1,3-dimethyl-7-phenyl-8-thio- (7CI, 8CI) (CA INDEX NAME)



L25 ANSWER 410 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1964:461824 CAPLUS
DOCUMENT NUMBER: 61:61824
ORIGINAL REFERENCE NO.: 61:10735f-g
TITLE: Heterocyclic steroids in the antiinflammatory series
AUTHOR(S): Mrozik, Helmut; Buchschacher, Paul; Hannah, John; Freid, John H.
CORPORATE SOURCE: Merck & Co. Inc., Rahway, NJ
SOURCE: Journal of Medicinal Chemistry (1964), 7(5), 584-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 61:61824
GI For diagram(s), see printed CA Issue.
AB A number of heterocyclic-fused steroids have been prepared as an extension of the lead provided by the steroidal [3,2-c]pyrazoles as antiinflammatory agents. The syntheses of steroidal [3,2-d]thiazoles, such as I, [2,3-d]imidazoles, [3,2-d]triazoles, and [3,2-d]pyrimidines related to cortisone are described. The 3'-phenyl[3,2-d]-3'H-1',2',3'-triazole function has been found to be a powerful activity-enhancing group.
IT **107225-48-9**, Dispiro[cyclopenta[7,8]phenanthro[2,3-d]imidazole-1(11H),4'-[1,3]dioxolane-5',4''-[1,3]dioxolan]-11-one, 2,3,3a,3b,4,5,7,10,10a,10b,12,12a-dodecahydro-8-mercapto-2,10a,12a-trimethyl-7-phenyl-
(preparation of)
RN 107225-48-9 CAPLUS
CN Dispiro[cyclopenta[7,8]phenanthro[2,3-d]imidazole-1(11H),4'-[1,3]dioxolane-5',4''-[1,3]dioxolan]-11-one, 2,3,3a,3b,4,5,7,10,10a,10b,12,12a-dodecahydro-8-mercapto-2,10a,12a-trimethyl-7-phenyl- (7CI) (CA INDEX NAME)



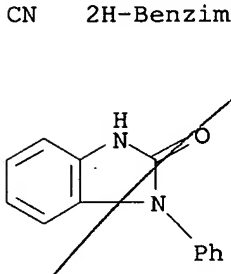
close art

L25 ANSWER 411 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1963:475287 CAPLUS
DOCUMENT NUMBER: 59:75287

ORIGINAL REFERENCE NO.: 59:13967h,13968a-b
TITLE: Benzimidazole derivatives. XIV. Amination of 1-cyclohexyland 1-phenylbenzimidazole
AUTHOR(S): Simonov, A. M.; Pozharskii, A. F.
CORPORATE SOURCE: State Univ., Rostov-on-Don
SOURCE: Zhurnal Obshchei Khimii (1963), 33(7), 2350-4
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. CA 59, 10024d. 5-Amino-1-cyclohexylbenzimidazole was diazotized in aqueous HCl, treated with KH2PO2 1 hr. with stirring and 1 day in the cold, and neutralized with NH4OH to give 70% 1-cyclohexylbenzimidazole (I), m. 87-9° (picrate m. 207-9°; methiodide m. 245°). Heated with NaNH2 in xylene 4 hrs., then kept 12 hrs. with H2O, I gave 2-amino1-cyclohexylbenzimidazole, m. 207-9°; 2-p-nitrobenzylidenimino derivative m. 194-5°. Heating urea with o-PhNHC6H4NH2.HCl 1-1.5 hrs. at 160-70° gave, after treatment with hot aqueous NaOH and neutralization of the filtrate, 100% 1-phenyl-2-hydroxybenzimidazole, m. 202-3.5°, which with POCl3 in Me2NCHO 7 hrs. at 150-60° in a sealed ampul gave 7% 1-phenyl2-chlorobenzimidazole, m. 67-8°. 1-Phenylbenzimidazole (II) and NaNH2 in xylene gave some MeNH2 and 57-68% 2-amino1-phenylbenzimidazole (III), m. 151-2° (picrate m. 251-3°), which gave an azomethine C13H11N3 with p-nitrobenzaldehyde. The residues, after isolation of this substance, gave 4-5% o-H2NC6H4NHPh; N-p-nitrobenzoyl derivative m. 181-3°. H and NaNH2 in PhNMe2 at 110-50° also gave MeNH2 and III in 3% yield; the latter gave a 2-p-nitrobenzoyl derivative, m. 247-8°, and a 2-p-nitrobenzylidenimino derivative, m. 198-200°. 2-Chloro1-phenylbenzimidazole and alc. NH3 15 hrs. at 150-60° gave 2-amino-1-phenylbenzimidazole isolated as the picrate in low yield.

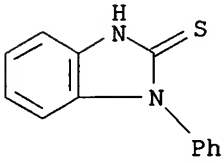
IT **14813-85-5**, 2-Benzimidazolol, 1-phenyl-
(preparation of)
RN 14813-85-5 CAPLUS
CN 2H-Benzimidazol-2-one, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



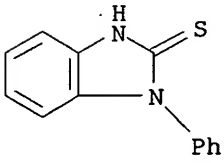
L25 ANSWER 412 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1963:420140 CAPLUS
DOCUMENT NUMBER: 59:20140
ORIGINAL REFERENCE NO.: 59:3582f-g
TITLE: Collecting action of some substituted 2-mercaptobenzimidazoles
AUTHOR(S): Tyurenkova, G. N.; Lipatova, L. F.; Postovskii, I. Ya.
SOURCE: Tsvetnye Metally (Moscow, Russian Federation) (1963), 36(2), 77-80
CODEN: TVMTAX; ISSN: 0372-2929
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Infrared spectrum examination showed that N-substituted mercaptobenzimidazoles (I), such as the N-phenyl derivative, both as a K salt and as a thiol, react to form Cu salts with the surface of the oxidized Cu minerals malachite and chrysocolla. The collecting action of I in flotation is attributed to its ability to become fixed on the mineral surface with the aid of the active SH group, making the surface hydrophobic.

IT **4493-32-7**, 2-Benzimidazolethiol, 1-phenyl-
(in flotation of oxidized Cu minerals)
RN 4493-32-7 CAPLUS
CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



IT **105791-76-2**, Copper, bis(1-phenyl-2-benzimidazolethiolato)-
(preparation of)
RN 105791-76-2 CAPLUS
CN Copper, bis(1-phenyl-2-benzimidazolethiolato)- (7CI) (CA INDEX NAME)



●1/2 Cu(II)

L25 ANSWER 413 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1963:81543 CAPLUS
DOCUMENT NUMBER: 58:81543
ORIGINAL REFERENCE NO.: 58:13965a-d
TITLE: Penicillanic and cephalosporanic acids
INVENTOR(S): Chow, Alfred W.; Hoover, John R. E.
PATENT ASSIGNEE(S): Smith Kline & French Laboratories
SOURCE: 29 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 617187		19621105	BE	
DE 1212089			DE	
GB 957570			GB	
US 3131184		1964	US	
US 3252971		1966	US	
PRIORITY APPLN. INFO.:			US	19610503

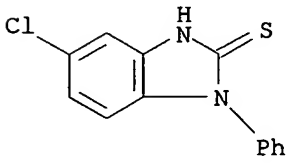
AB Carboxylic acid derivs. of heterocyclic compds. are treated with penicillanic and cephalosporanic acids to give amides which are not toxic and have pharmaceutical applications. 3-Phenyl-2-benzo[b]thiophenecarboxylic acid (5.2 g.) and 11 ml. SOCl2 is kept at room temperature overnight to give 4 g. oil, the oil dissolved in 50 ml. Me2CO, the solution added to 4.3 g. 6-aminopenicillanic acid in 190 ml. 3% NaHCO3 and 120 ml. Me2CO, the mixture kept 1.5 hrs. at 25°, extracted twice with 150 ml. Et2O, the aqueous phase mixed with 40 ml. BuOAc, the mixture cooled to below 10°, 20% H3PO4 is added to pH 2.4, the 2 phases that form are

separated, the aqueous phase is extracted with 15 ml. BuOAc, the BuOAc extract washed with 10 ml. H2O, the pH adjusted to 3, 9.6 ml. 30% K 2-ethylhexanoate in iso-PrOH added, Et2O added, and the mixture cooled to give a precipitate which is washed with 1:1 Et2O-BuOAc. The precipitate (1 g.) is dissolved in H2O and treated with dilute HCl at 5° to give 6-(3-phenyl-2-benzo[b]thiophenecarbonylamino)penicillanic acid. Similarly prepared are 6-(3-phenylindole-2-carbonylamino)penicillanic acid, 7-(3-phenyl-2-benzo[b]thiophenecarbonylamino)cephalosporanic acid, internal salt of 3-pyridiniummethyl-7-(3-phenyl-2-benzo[b]thiophenecarbonylamino)decephalosporanic acid, 3-propionyloxymethyl-7-(3-phenyl-2-benzo[b]thiophenecarbonylamino)decephalosporanic acid, 3-methyl-7-(3-phenyl-2-benzo[b]thiophenecarbonylamino)decephalosporanic acid, N-ethylpiperidine salt of 6-(2-phenyl-3-benzo[b]thiophenecarbonylamino)penicillanic acid, Et3N salt of 6-(3-phenyl-2-benzo[b]thiophenecarbonylamino)penicillanic acid, and the salt from (PhCH2)2NCH2CH2NH2 and 6-(2-phenyl-3-benzo[b]thiophenecarbonylamino)penicillanic acid.

IT **96459-92-6**, 2-Benzimidazolethiol, 5-chloro-1-phenyl- (preparation of)

RN 96459-92-6 CAPLUS

CN 2-Benzimidazolethiol, 5-chloro-1-phenyl- (6CI, 7CI) (CA INDEX NAME)



L25 ANSWER 414 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1963:59732 CAPLUS

DOCUMENT NUMBER: 58:59732

ORIGINAL REFERENCE NO.: 58:10190b-e

TITLE: Reaction of carbanilides with sodium hypochlorite

AUTHOR(S): Oftedahl, Marvin L.; Radue, Robert W.; Dietrich, Martin W.

CORPORATE SOURCE: Monsanto Chem. Co., St. Louis, MO

SOURCE: Journal of Organic Chemistry (1963), 28, 578-80
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 58:59732

GI For diagram(s), see printed CA Issue.

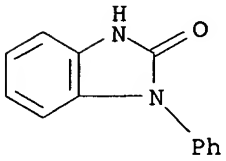
AB The behaviour of 3,4,4'-trichlorocarbanilide (I) on treatment with hypochlorite was investigated. Carbanilide (10.6 g.) in 300 ml. MeOH treated in the cold with 4 g. NaOH in 15 ml. H2O, then treated in the cold with 110 ml. 1.36M NaOCl solution, left 0.5 hr., neutralized, evaporated, and the residue collected gave 6 g. 1-phenyl-6-chloro-2-benzimidazolinone (II), m. 264-7° (PhMe). Acetylation of 1 g. II gave 70% of the monoacetate, m. 160.0-160.5°. Carbanilide (10.6 g.) when treated with 45 ml. 1.23M NaOCl gave 71% 1-phenyl-2-benzimidazolinone, m. 203.5-4.0°; monoacetate (90% yield) m. 134-5°. Treatment of I gave 39% 1-(3,4-dichlorophenyl)-6-chloro-2-benzimidazolinone (III), m. 259-60°; monoacetate (65%) m. 164-5°. Treatment of 3,4-dichlorocarbanilide (IIIa) with 3 moles of hypochlorite gave 13.7% III. 3,3',4,4'-Tetrachlorocarbanilide treated as above was recovered in 75% yield. 1-Ethyl-1-(4-chlorophenyl)-3-(3,4-dichlorophenyl)urea and

1-methyl-1-(3,4-dichlorophenyl)-3-(4-chlorophenyl)urea (IV) similarly treated with 3 moles of hypochlorite gave a recovery of 80% and 86%, resp., of starting material. IV was obtained by treatment of N-methyl-3,4-dichloroaniline with p-chlorophenyl isocyanate in Et2O, m. 159-60°. The direction of ring closure of both I and III suggested that the cyclization proceeded via intramol. attack of an electrophilic N upon the most electron rich aryl ring available. Failure of the last three compds. to cyclize may be explained by reduction of the electron density of both aryl rings, thus preventing attack by electrophilic N.

IT **14813-85-5**, 2-Benzimidazolinone, 1-phenyl- **40160-01-8**, 2-Benzimidazolinone, 1-acetyl-5-chloro-3-phenyl- **54986-47-9**, 2-Benzimidazolinone, 6-chloro-1-phenyl- **77037-61-7**, 2-Benzimidazolinone, 6-chloro-1-(3,4-dichlorophenyl)- **78162-50-2**, 2-Benzimidazolinone, 1-acetyl-3-phenyl- **92424-42-5**, 2-Benzimidazolinone, 1-acetyl-5-chloro-3-(3,4-diohlorophenyl)- (preparation of)

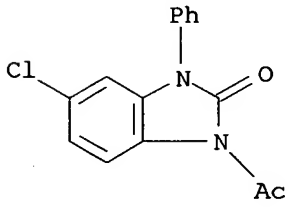
RN 14813-85-5 CAPLUS

CN 2H-Benzimidazol-2-one, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



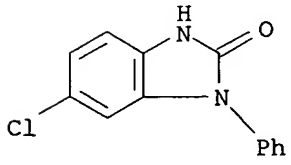
RN 40160-01-8 CAPLUS

CN 2H-Benzimidazol-2-one, 1-acetyl-5-chloro-1,3-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



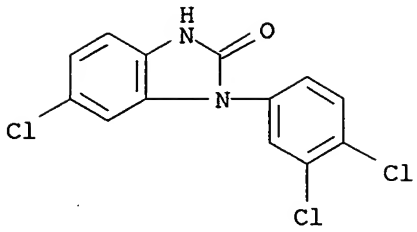
RN 54986-47-9 CAPLUS

CN 2H-Benzimidazol-2-one, 6-chloro-1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)

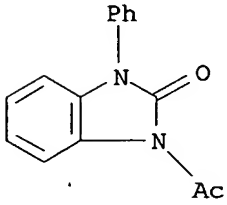


RN 77037-61-7 CAPLUS

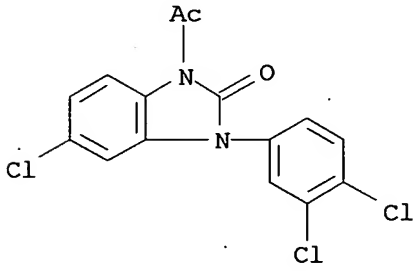
CN 2H-Benzimidazol-2-one, 6-chloro-1-(3,4-dichlorophenyl)-1,3-dihydro- (9CI) (CA INDEX NAME)



RN 78162-50-2 CAPLUS
CN 2H-Benzimidazol-2-one, 1-acetyl-1,3-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



RN 92424-42-5 CAPLUS
CN 2-Benzimidazolinone, 1-acetyl-5-chloro-3-(3,4-dichlorophenyl)- (7CI) (CA INDEX NAME)



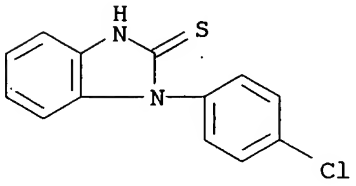
L25 ANSWER 415 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1962:38475 CAPLUS
DOCUMENT NUMBER: 56:38475
ORIGINAL REFERENCE NO.: 56:7303c-e
TITLE: N-Substituted derivatives of benzimidazole and their flotation properties
AUTHOR(S): Tyurenkova, G. N.; Silina, E. I.; Postovskii, I. Ya.
SOURCE: Zhurnal Prikladnoi Khimii (Sankt-Peterburg, Russian Federation) (1961), 34, 2327-31
CODEN: ZPKHAB; ISSN: 0044-4618
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. CA 54, 4147b.-To determine the flotation properties (F.P.) of substituted 2-mercaptobenzimidazoles (I) and to correlate the F.P. with the structure the following derivs. of I were obtained by the reaction ClC6H4NO2 + RNH2 at 200-20° in the presence of NaOAc followed by reduction with SnCl2 in HCl and treatment with CS2 and C5H5N to give II (R, % yield, and m.p. given): Me, 60, 187-9°; n-C4H9, 66, 104°; HOCH2, 67, 185°; Ph, 80, 196°; p-MeC6H4, 61, 246-8°; p-MeOC6H4,

38, 212-14°; p-ClC6H4, 77, 251-3°. The F.P. of these derivs. were determined with mixts. of quartz and galenite, cerussite, or malxite. The results were given in terms of 2-mercaptobenzothiazole as a standard. The results indicated a parallelism between the increase in the F.P. and the increase in the dimensions of the hydrophobic group.

IT **3387-19-7**, 2-Benzimidazolethiol, 1-(p-chlorophenyl)-
4493-32-7, 2-Benzimidazolethiol, 1-phenyl- **26495-07-8**,
2-Benzimidazolethiol, 1-(p-methoxyphenyl)- **92149-91-2**,
2-Benzimidazolethiol, 1-p-tolyl-
(preparation of)

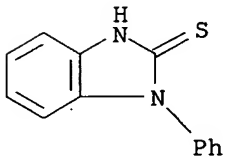
RN 3387-19-7 CAPLUS

CN 2H-Benzimidazole-2-thione, 1-(4-chlorophenyl)-1,3-dihydro- (9CI) (CA INDEX NAME)



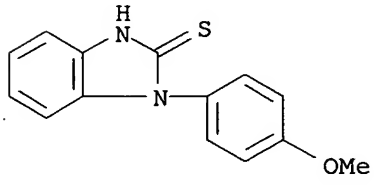
RN 4493-32-7 CAPLUS

CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



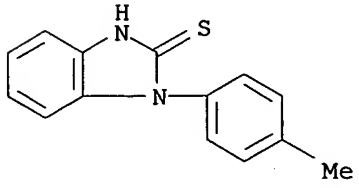
RN 26495-07-8 CAPLUS

CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 92149-91-2 CAPLUS

CN 2-Benzimidazolethiol, 1-p-tolyl- (7CI) (CA INDEX NAME)



L25 ANSWER 416 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1961:104300 CAPLUS
DOCUMENT NUMBER: 55:104300
ORIGINAL REFERENCE NO.: 55:19566i,19567a-b
TITLE: Improving the adhesion of greasy printing inks to photographic silver images
INVENTOR(S): Gunther, Eberhard; Lassig, Wolfgang
PATENT ASSIGNEE(S): Agfa Akt.-Ges.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

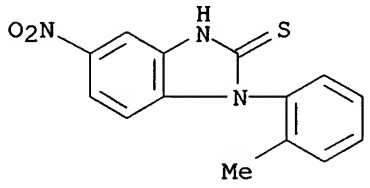
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1064343		19590827	DE	

AB The adhesion of greasy printing inks to photographic Ag images, especially those produced on the surface of a hydrophilic layer, is improved by partial oxidation of the surface of the image and reaction of the resulting Ag ions with organic mercapto derivs. Thus, on H2O-resistant paper, coated on both sides with a lacquer and provided on 1 side with a gelatin layer containing nuclei of Ag or other noble metals or their derivs., a Ag is produced by the Ag salt-diffusion method. The paper is washed, treated with 5% aqueous K2Cr2O7, washed, and immersed for 20 sec. in 1000 cc. solution containing 20 g. EtOCS2K and 20 cc. 2N NaOH to yield a printing plate which can be used for printing up to 500 copies. The oxidation of the Ag image can also be achieved with 1% aqueous KMnO4. Examples are given for the use of C18H37SH, C18H37NHCONHNHCS2Me, PhNHCSNH2, 1-amino-2-mercapto-5-heptadecyl-1,3,4-triazole (I), 5-PhCH2 analog of I, 2-mercapto-5-octadecylthio-1,3,4-triazole, Et2NCS2Na, 2-mercapto-1-(o-tolyl)-5-nitrobenzimidazole, and 1-(p-nitrobenzylideneamino)-2-mercapto-1,3,4-triazole.

IT **100541-52-4**, 2-Benzimidazolethiol, 5-nitro-1-o-tolyl- (photographic image treatment with, for greasy-ink adhesion improvement)

RN 100541-52-4 CAPLUS

CN 2-Benzimidazolethiol, 5-nitro-1-o-tolyl- (6CI) (CA INDEX NAME)



L25 ANSWER 417 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1961:99557 CAPLUS
DOCUMENT NUMBER: 55:99557
ORIGINAL REFERENCE NO.: 55:18782f-i,18783a-i,18784a-d
TITLE: Purines
INVENTOR(S): Roch, Josef
PATENT ASSIGNEE(S): Dr. Karl Thomae G. m. b. H.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

	GB 864145	19610329	GB
	DE 1115260		DE
	US 3016378	1962	US

AB New purines were prepared, having 2 or 3 substituted amino groups attached to the nucleus, at least 1 of which was an N-heterocyclic group. The compds. had valuable pharmacol. properties, such as coronary expanding effect, hypotensive action, respiratory control action, and analgesic, sedative, and antipyretic properties. Piperidine (20 cc.) added with stirring to 9.5 g. 2,6,8-trichloro-7-methylpurine in 100 cc. dioxane, the mixture heated to boiling, cooled, and poured into 350 cc. H2O gave 10.2 g. 2-chloro-6,8-dipiperidino-7-methylpurine, m. 140-2° (MeOH). The following purines were prepared (compound, % yield, and m.p. given): 2-chloro-6,8-dimorpholino-7-methylpurine, 75, 284-6°; 2-chloro-6-morpholino-8-benzylamino-7-methylpurine, 86, 211-13° (MeOH) (from 2,6-dichloro-8-benzylamino-7-methylpurine, m. 226-8°); 2-chloro-6-hydrazino8-morpholino-7-methylpurine, decomposed above 250°; 2-chloro-6-hydrazino-8-piperidino-7-methylpurine. 57, decomposed at 250°; 2-chloro-6-(-methoxypropylamino)-8 piperidino-7-methylpurine, 81, 114-16°; 2-chloro-6-guanidino-8-piperidino-7-methylpurine, 89, 130-2°; 2-chloro-6-diethylamino-8-piperidino-7-methylpurine, 98, 108-10° (MeOH); 2-chloro-6-(γ-dimethylaminopropylamino)-8-piperidino-7-methylpurine, 81, 91-3°; 2,6,8-trimorpholinopurine, 48, 247-8° (decomposition) (MeOH); 2-morpholino-6,8-bis(methylamino)-7-methylpurine, 84, 307-9° (decomposition) [from 2-chloro-6,8-bis(methylamino)-7-methylpurine, m. 247-9°]; 2-morpholino-6,8-bis(dimethylamino)-7-methylpurine, 84, 195-7° (H2O); 2,6,8-trimorpholino-7-methylpurine, 81, 238.5-9.5° (H2O); 2-morpholino-6,8-diperidino-7-methylpurine, 95, 189-90°; 2-pyrrolidino-6,8-dimorpholino-7-methylpurine, 89, 197-9°; 2-methylethanolamino-6,8-dimorpholino-7-methylpurine, 64, 148-50° (H2O); 2,8-dimorpholino-6-hydrazino-7-methylpurine, 42, 221-3° (MeOH); 2-(β-hydroxyethylamino)-6,8-dipiperidino-7-methylpurine, 80, 220-2°; 2-morpholino-6-diethylamino-8-piperidino-7-methylpurine, 78, 191-3° (MeOH); 2,6-dimorpholino-8-piperidino-7-methylpurine, 93, 209-11° (EtOH-H2O) (from 2,6-dichloro-8-piperidino-7-methylpurine, m. 143-5°); 2,6-dimorpholino-8-anilino-7-methylpurine, 81, 240-2° (HCONMe2-H2O); 2,6-dimorpholino-8-benzyl-amino-7-methylpurine, 84, 197-9°; 2,6-dimorpholino-7-methylpurine, 84, 215-17°; 2,6-dipiperidino-7-methylpurine, 82, 176-8° (petr. ether-C6H6); 2,6-dimorpholino-8-hydroxypurine, 76, above 350°; 2-ethylthio-6,8-dimorpholino-7-methylpurine, -, 188-90°; 2-(β-ethoxyethoxy)-6,8-dimorpholino-7-methylpurine, 61, 134-6° (petr. ether-C6H6); 2,6,8-trimorpholino-7-methylpurine, 79, 238-40° (H2O) [from 2-chloro-6,8-diiodo-7-methylpurine, m. 239-41° (MeOH)]; 2,6,8-trimorpholino-9-phenylpurine, 63, 223-4° (MeOH); 2,6-dipiperidino-8-hydroxy-9-phenylpurine, 96, 206° (EtOH-dioxane); 2,6,8-trimorpholino-7-methylpurine, 75, 238-40° (H2O); 2,6,8-tripiperidino-7-methylpurine, 91, 216-18° (MeOH); 2,6-dimorpholino-8-phenylpurine, 55, 244-5° (MeOH); 2,6-dimorpholino-8-benzylpurine, 53, 224° (MeOH-H2O); 2-phenylthio-6,8-dimorpholino-7-methylpurine, 71, 100-2° (MeOH); 2-phenoxy-6,8-dimorpholino-7-methylpurine, 87, 192-4° (MeOH); 2,6,8-trimorpholino-9-benzylpurine, -, 162-3° [from 2,6,8-trichloro-9-benzylpurine, m. 126-8° (MeOH)]; 2,6-dimorpholino-8-hydroxy-9-(p-chlorophenyl)purine, 24, 346-8° (dioxane-EtOH); 2,6-dimorpholino-8-hydroxy-9-(p-methoxyphenyl)-purine, 15, above 350°; 2,6-dipiperidino-8-hydroxy-9-(p-tolyl)purine, 51, 316-18°; 2,8-dimorpholino-6-piperidino-7-methylpurine, 58, 207-9° (MeOH-H2O) (from 2-chloro-8-morpholino-6-piperidino-7-methylpurine, m. 224-6°, obtained from 2,6-dichloro-8-morpholino-7-methylpurine, m. 193-4°); 2-piperidino-6,8-dimorpholino-7-methylpurine, 82, 190-2° (petr. ether-C6H6); 2,6-dipiperidino-8-morpholino-7-methylpurine, 53, 197-9° (MeOH-H2O);

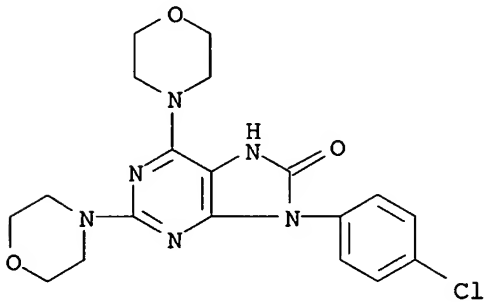
2,6-dipiperidino-9-amino-7-methylpurine, 97, 230-2°;
2,6-dimorpholino-8-(N-phenylpiperazino)-7-methylpurine, 93, 226-8°;
2-[N-(p-chlorophenyl)piperazino]-6,8-dimorpholino-7-methylpurine, 79,
227-30°; 2,6-dimorpholino-8-hexa-methylenimino-7-methylpurine, 75,
159-61°; 2-hexamethylenimino-6,8-dimorpholino-7-methylpurine, 92,
200-2°; 2-chloro-6,8-dimorpholino-9-(p-tolyl)purine, 88,
197-8°; 2,8-dimorpholino-6-thio-7-methylpurine, 42, 255-7°;
2-ethoxy-6,8-dipiperidino-7-methylpurine, 53, 134-5°;
2-dimethylamino-6,8-dimorpholino-7-methylpurine, 94, 167-9°;
2,6-dimorpholino-8-(morpholinomethyl)purine, 46, 235-7°;
2,6-dimorpholino-8-hydroxy-7-methylpurine, 81, 271-3°;
2,6-dipiperidino-8-hydroxy-7-methylpurine, 82, 231-3°;
2-morpholino-6-diethylamino-8-hydroxy-7-methylpurine, 57, 182-4°;
2-morpholino-6-piperidino-8-hydroxy-7-methylpurine, 75, 248-50°;
2,6-dimorpholino-8-chloropurine, 72, 308° (decomposition);
2-chloro-6,8-bis(N-phenylpiperazino)-7-methylpurine, 75, 120°;
2-chloro-6-piperidino-8-morpholino-7-methylpurine, 86,237-9°;
2-chloro-6-morpholino-8-(p-chloroanilino)-7-methylpurine, 90,
147-9°; 2-chloro-6,8-dimorpholino-9-methylpurine, 81,
213-16°; 2-chloro-6,8-dipiperidino-9-methylpurine, 67,
162-3°; 2-methylethanolamino-6,8-dipiperidino-7-methylpurine, 83,
180-2°; 2-morpholino-6,8-bis(N-phenylpiperazino)-7-methylpurine,
53, 156-8°; 2,6,8-trimorpholino-8-methylpurine, 62,
249-50°; 2,6,8-tripiperidino-9-methylpurine, 62, 135-7°;
2-piperidino-6,8-dimorpholino-9-methylpurine, 92, 188-9°;
2,8-dipiperidino-6-morpholino-9-methylpurine, 83, 129-30°;
2-morpholino-6,8-dipiperidino-9-methylpurine, 90, 134-5°;
2,8-dimorpholino-6-piperidino-9-methylpurine, 98, 169-71°;
2,6-dipiperidino-8-(β-hydroxyethylamino)-7-methylpurine, 94,
191-3°; 2,6-dimorpholino-8-benzylmethylamino-7-methylpurine, 95,
163-5°; 2,6-dimorpholino-8-(β-hydroxyethylamino)-7-
methylpurine, 81, 223-5°; 2,8-dimorpholino-6-piperidinopurine, 76,
200-2°; 2,6,8-trimorpholino-7-benzylpurine, 92, 224-6°;
2,8-dimorpholino-6-(N-methylpiperazino)purine, 79,257-8°;
2,6,8-trimorpholino-7-(morpholinoethyl)purine, 64, 212-13°; 2,
6-dimorpholino-8-(N-methylpiperazino)purine, 71, 235-6°;
2,6-dipiperidino-8-benzylmethylamino-7-methylpurine, 86, 160-2°;
2-benzylmethylamino-6,8-dipiperidino-7-methylpurine, 81, 153-5°;
2-(N-methylpiperazino)-6,8-dipiperidino-7-methylpurine, 89, 183-5°;
2-(N-methylpiperazino)-6,8-dimorpholino-7-methylpurine, 61,
209-11°; 2-chloro-6,8-di(hexamethylenimino)-7-methylpurine, 68,
170-2°; 2-chloro-6,8-dipyrrolidino-7-methylpurine, 86,
218-20°; 2-diethanolamino-6,8-dipiperidino-7-methylpurine,
52,195-6°; 2-isopentylamino-6,8-dipiperidino-7-methylpurine, 63,
189-90°; 2,6-dipyrrolidino-8-allylamino-7-methylpurine, 93,
213-15°; 2-(β,γ-dihydroxypropylamino)-6,8-dipiperidino-
7-methylpurine, 70, 242-4°; 6,8-dimorpholino-7-methylpurine, 41,
251-2°; 2-hydroxy-6-methylamino-8-piperidino-7-methylpurine, 56,
260° (decomposition); 2,6-dimorpholino-8-cyclohexylamino-7-methylpurine,
69, 148-50°; 2,8-dimorpholino-6-anilinopurine, 78, 162-3°;
2,8-dimorpholino-8-aminopurine, 84, 278-9°; 2,8-dimorpholino-6-
(diethanolamino)purine, 70, 252-3°; 2,8-dipiperidino-6-(β-
hydroxyethylamino)purine, 84, 163-5°; 2-methylcyclohexylamino-6,8-
dimorpholino-7-methylpurine, 76, 231-3°; 2-amino-6-morpholino-8-
chloropurine, 66, 300° (decomposition); 2,8-dimorpholino-6-
benzylaminopurine-HCl, 61, 226-7°; 2,8-dianilino-6-piperidinopurine-
HCl, 87, 300° (decomposition); 2,8-dipiperidino-6-
(diethanolamino)purine, 72, 88-90°; 2,8-dimorpholino-6-
hydroxypurine, 66, 300° (decomposition); 2,8-dimorpholino-6-
ethoxypurine, 69, 252-5°; 2-benzoyloxy-6,8-dimorpholino-7-
methylpurine, 58, 213-15°; 2,6-bis(3-methoxypropylamino)-8-
morpholinopurine, 73, 204-5°; 2-morpholino-6,8-bis(allylamino)-7-
methylpurine, 68, 206-7°; 2,6-dimorpholino-8-(β-

diethylaminoethylamino)-7-methylpurine, 65, 114-15°;2,6-dimorpholino-8-(3-methoxypropylamino)-7-methylpurine, 59, 104-6°; 2,6,8-tris(3-methylpiperidino)-7-methylpurine, 78, 70-2°; 2-morpholino-6,8-bis(cyclohexylamino)-7-methylpurine, 97, 247-9°; 2,6,8-tris(4-methylpiperidino)-7-methylpurine, 67, 210-11°.

IT **102176-98-7**, 9H-Purin-8-ol, 9-(p-chlorophenyl)-2,6-dimorpholino-
102471-79-4, 9H-Purin-8-ol, 9-phenyl-2,6-dipiperidino-
102472-89-9, 9H-Purin-8-ol, 2,6-dipiperidino-9-p-tolyl-
(preparation of)

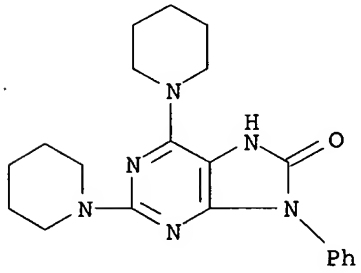
RN 102176-98-7 CAPLUS

CN 9H-Purin-8-ol, 9-(p-chlorophenyl)-2,6-dimorpholino- (6CI) (CA INDEX NAME)



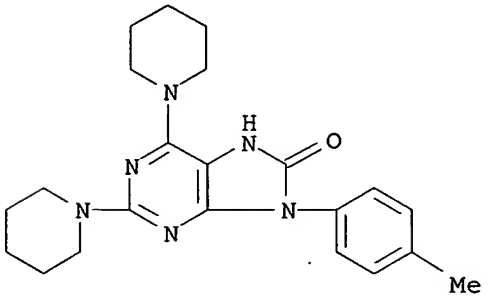
RN 102471-79-4 CAPLUS

CN 9H-Purin-8-ol, 9-phenyl-2,6-dipiperidino- (6CI) (CA INDEX NAME)



RN 102472-89-9 CAPLUS

CN 9H-Purin-8-ol, 2,6-dipiperidino-9-p-tolyl- (6CI) (CA INDEX NAME)



L25 ANSWER 418 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1961:83829 CAPLUS

DOCUMENT NUMBER: 55:83829

ORIGINAL REFERENCE NO.: 55:15846c-g

TITLE: Remedy for trichophyton
INVENTOR(S): Nakajima, Shotaro; Tanaka, Ichiro; Aka, Teruya; Yasushige, Hisao
PATENT ASSIGNEE(S): Taisho Drug Manufg. Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 35017036		19601117	JP	

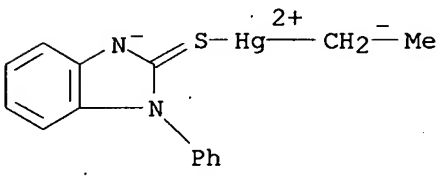
GI For diagram(s), see printed CA Issue.

AB x-RC6H3.NH.C(SH):N (I, R = H or Cl) and BrHgR' (II, R' = alkyl) are treated in KOH to give x-RC6H3.N(HgR').C(SHgR'):N (III), or I and PhHgOAc are treated in KOH to give x-RC6H3.N(HgPh).C(SHgPh):N (IV), or x-RC6H3.NPh.C(SH):N and II are treated in KOH to give x-RC6H3.NPh.C(SHgR'):N (V), or x-RC6H3.NH.C(SR'):N (VI) and II are treated in KOH to give x-RC6H3.N(HgR').C(SR'):N (VII). Thus, 1.8 g. VI (R = H, R' = Et) in 50 ml. alc. treated with 3 g. II (R' = Et), the solution filtered and the filtrate made up to 200 ml. with H2O gave 3.3 g. VII (R = H, R' = Et), m. 128-9° (70% alc.). Similarly are prepared x-RC6H3.NR'.C(SR''):N, where [R, R', R'', m.p., and the min. growth inhibitory dilution for Trichophyton interdigitale (1000 dilution = 1) are given]: H, EtHg, Et, 128-9°, 2920; H, Ph, EtHg, 114-15%, 1950; H, EtHg, EtHg, 253-4° (decomposition), 2920; H, PrHg, PrHg, 216-17°, 2920; H, BuHg, BuHg, 193-4°, 2900; H, C9H9Hg, C9N9Hg, 143-53°, 20; H, PhHg, PhHg, above 300%,130; Cl, EtHg, EtHg, 228-30° (decomposition), 2920; Cl, PrHg, PrHg, 209-20.5°, 110; Cl, BuHg, BuHg, 194-5°, 260; Cl, PhHg, PhHg, 258° (decomposition), 170; H, Ph, PrHg, 71-2°, 2920.

IT **59547-63-6**, Benzimidazole, 2-(ethylmercurithio)-1-phenyl- (fungicide)

RN 59547-63-6 CAPLUS

CN Mercury, (1,3-dihydro-1-phenyl-2H-benzimidazole-2-thionato-S)ethyl- (9CI) (CA INDEX NAME)



L25 ANSWER 419 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1961:81686 CAPLUS
DOCUMENT NUMBER: 55:81686
ORIGINAL REFERENCE NO.: 55:15467e-h
TITLE: Benzimidazole derivatives. V. Action of bases on salts of N-arylbenzimidazolium group
AUTHOR(S): Simonov, A. M.; Vitkevich, N. D.; Zheltonozhko, S. Ya.
CORPORATE SOURCE: State Univ., Rostov
SOURCE: Zhurnal Obshchei Khimii (1960), 30, 2684-8
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

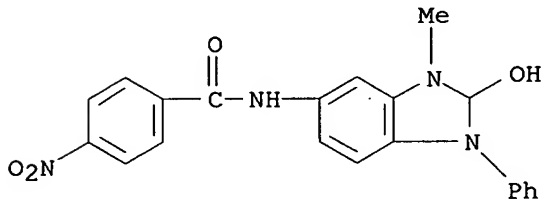
AB cf. CA 54, 9896a, 24677i. 1,2-Dimethyl-3-(2,4-dinitrophenyl)-benzimidazolium benzenesulfonate with aqueous NH4OH gave 90% red 2-(N-acetylmethylamino)-2',4'-dinitrodiphenylamine, m. 168-9°; heated to 125° this passed into a yellow form, also m.

168-9°. Prolonged heating in 1:1 HCl gave 2-methylamino-2',4'-dinitrodiphenylamine, m. 178°, which heated with Ac2O 1 hr. reverted to the above Ac derivative o-Aminodiphenylamine and HCO2H gave 1-phenylbenzimidazole, m. 96.5°, which heated with 2,4-(O2N)2C6H3Cl 2.5 hrs. at 100° gave 60% yellow 2-(N-formylphenylamino)-2',4'-dinitrodiphenylamine, m. 200-1°, which with alc. HCl in 15 hrs. refluxing gave 90% red 2-phenylamino-2',4'-dinitrodiphenylamine, m. 170-70.5°. 5-Amino-1-phenylbenzimidazole and p-O2NC6H4COCl in aqueous EtOH-NaHCO3 gave in 2-3 hrs. 92% 5-(p-nitrobenzamido)-1-phenylbenzimidazole, m. 258-9°, whose Me p-toluenesulfonate (I), m. 263-4°, with picric acid gave 5-(p-nitrobenzamido)-3-methyl-1-phenylbenzimidazolium picrate, m. 213-14°. I and aqueous Na2CO3 gave a precipitate of orange pseudo base, C21H18O4N4, m. 197-8°, which in hot HCl gave a precipitate containing Cl ion; treated with bases this yielded the pseudo base; the chloride, m. 299-300°, yielded the picrate. Benzimidazole and picryl chloride in EtOH at 60° gave 1-picrylbenzimidazole, m. 211-12°, which with PhSO3Me gave 35% green-yellow 1-methyl-3-picrylbenzimidazolium benzenesulfonate, m. 243-4°. 1-Phenylbenzimidazole did not form a stable dinitrochlorophenylate after being fused with dinitrochlorobenzene.

IT **102312-13-0**, 2-Benzimidazolinol, 3-methyl-5-p-nitrobenzamido-1-phenyl-
(preparation of)

RN 102312-13-0 CAPLUS

CN 2-Benzimidazolinol, 3-methyl-5-p-nitrobenzamido-1-phenyl- (6CI) (CA INDEX NAME)



L25 ANSWER 420 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1961:22770 CAPLUS

DOCUMENT NUMBER: 55:22770

ORIGINAL REFERENCE NO.: 55:4507f-i,4508a-b

TITLE: Antispasmodic compounds

AUTHOR(S): Sabata, B. K.; Tripathy, P. B.; Rout, M. K.

CORPORATE SOURCE: Ravenshaw College, Cuttack

SOURCE: Proceedings of the Institution of Chemists (India) (1960), 32, 147-50
CODEN: PCHIA2; ISSN: 0369-8599

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

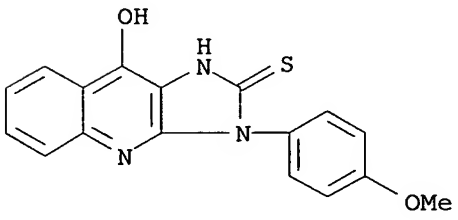
AB Compds. prepared by the method of Pujari and R. (CA 50,295a) were: 3-(4-ethoxyphenyl)-2-thiohydantoin (I), m. 122-3°, yield 80%; 3-(2-ethoxyphenyl)-2-thiohydantoin, m. 132°, yield 78%; 3-(4-methoxyphenyl)-2-thiohydantoin, m. 208°, yield 75%; 3-(4-bromophenyl)-2-thiohydantoin, m. 238°, yield 75%; 3-(1-naphthyl)-2-thiohydantoin, m. 176°, yield 78%. 3-(4-Ethoxyphenyl)-5-(2-nitrobenzylidene)-2-thiohydantoin (II), prepared in 70% yield by refluxing 2.5 hrs. a solution of 0.6 g. 2-nitrobenzaldehyde, 1 g. I, and 1.3 g. fused NaOAc in 15 ml. glacial HOAc, m. 165° (alc.). Compds. prepared similarly were: 3-(2-ethoxyphenyl)-5-(2-nitrobenzylidene)-2-thiohydantoin, m. 123°, yield 72%:

3-(4-methoxyphenyl)-5-(2-nitrobenzylidene)-2-thiohydantoin, m. 205°, yield 70%; 3-(4-bromophenyl)-5-(2-nitrobenzylidene)-2-thiohydantoin, m. 191-2°, yield 70%; and 3-(1-naphthyl)-5-(2-nitrobenzylidene)-2-thiohydantoin, m. 203°, yield 65%. III (R = p-EtOC6H4, R' = H), m. 203° (decomposition), was prepared in 65% yield by refluxing 1.5 g. II in 20 ml. glacial HOAc with Zn dust until the mixture was nearly colorless. Other III prepared similarly were (R, R', m.p., and % yield given): o-EtOC6H4, H, 159°, 68; p-MeOC6H4, H, 250°, 60; p-BrC6H4, H, 162°, 60; and 1-C10H7, H, 194°, 65. III (R = p-EtOC6H4, R' = OH), m. 128-9° (alc.), was prepared in 60% yield by fusing 2 g. I and 1.3 g. anthranilic acid (IV) at 150-60°, adding 1.23 g. finely powdered anhydrous NaOAc during 1 hr., and heating 4-5 hrs. The cooled mass was treated with NaHCO3 solution to remove unreacted IV and the residue dissolved in alkali. The filtrate, on acidification gave the product. III prepared similarly were (R, R', m.p., and % yield given): o-MeOC6H4, OH, 141-2°, 65; p-MeOC6H4, OH, 143°, 58; p-BrC6H4, OH, 224°, 59; and 1-C10H7, OH, 108°, 60. Quinolino[2',3':4,5]thiazolidin-2-one, m. 247°, was prepared in 68% yield by reducing a solution of 5-(2-nitrobenzylidene)-2,4-thiazolidinedione [prepared by condensing 2,4-thiazolidinedione (V) with 2-nitrobenzaldehyde] with Zn dust. 4'-Hydroxyquinolino[2',3':4,5]thiazolidin-2-one, m. 129°, was prepared in 60% yield by fusing V with 1.2 moles IV in the presence of fused NaOAc.

IT **109564-20-7**, 2H-Imidazo[4,5-b]quinoline-2-thione, 1,3-dihydro-9-hydroxy-3-(p-methoxyphenyl)- **109615-50-1**, 2H-Imidazo[4,5-b]quinoline-2-thione, 1,3-dihydro-3-(p-methoxyphenyl)- **110554-20-6**, 2H-Imidazo[4,5-b]quinoline-2-thione, 1,3-dihydro-3-(1-naphthyl)- **110554-21-7**, 2H-Imidazo[4,5-b]quinoline-2-thione, 1,3-dihydro-9-hydroxy-3-(1-naphthyl)- **113013-54-0**, 2H-Imidazo[4,5-b]quinoline-2-thione, 3-[p-ethoxyphenyl]-1,3-dihydro-9-hydroxy- **113062-66-1**, 2H-Imidazo[4,5-b]quinoline-2-thione, 3-[o-ethoxyphenyl]-1,3-dihydro-9-hydroxy- **113136-38-2**, 2H-Imidazo[4,5-b]quinoline-2-thione, 3-[o-ethoxyphenyl]-1,3-dihydro- **113184-50-2**, 2H-Imidazo[4,5-b]quinoline-2-thione, 3-[p-ethoxyphenyl]-1,3-dihydro- **131409-17-1**, 2H-Imidazo[4,5-b]quinoline-2-thione, 3-(p-bromophenyl)-1,3-dihydro-9-hydroxy- **131409-44-4**, 2H-Imidazo[4,5-b]quinoline-2-thione, 3-(p-bromophenyl)-1,3-dihydro-
(preparation of)

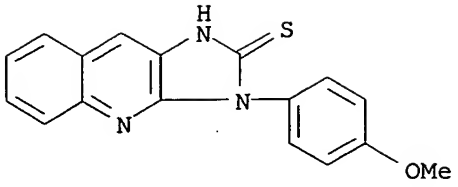
RN 109564-20-7 CAPLUS

CN 2H-Imidazo[4,5-b]quinoline-2-thione, 1,3-dihydro-9-hydroxy-3-(p-methoxyphenyl)- (6CI) (CA INDEX NAME)

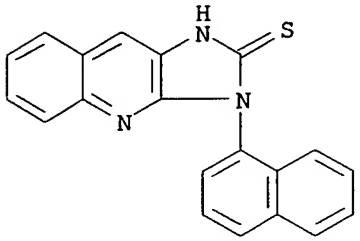


RN 109615-50-1 CAPLUS

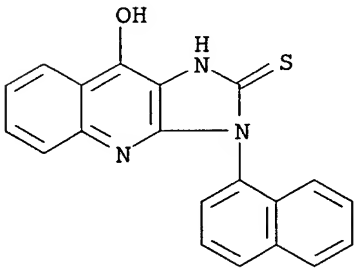
CN 2H-Imidazo[4,5-b]quinoline-2-thione, 1,3-dihydro-3-(p-methoxyphenyl)- (6CI) (CA INDEX NAME)



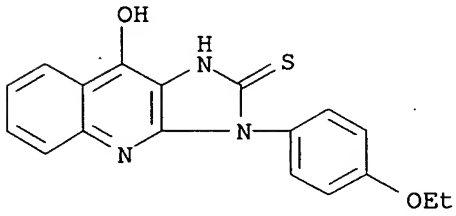
RN 110554-20-6 CAPLUS
CN 2H-Imidazo[4,5-b]quinoline-2-thione, 1,3-dihydro-3-(1-naphthyl)- (6CI) (CA INDEX NAME)



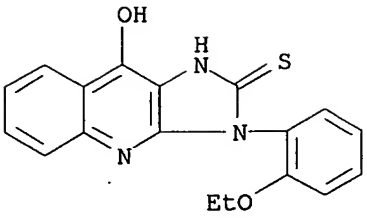
RN 110554-21-7 CAPLUS
CN 2H-Imidazo[4,5-b]quinoline-2-thione, 1,3-dihydro-9-hydroxy-3-(1-naphthyl)- (6CI) (CA INDEX NAME)



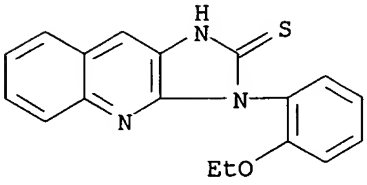
RN 113013-54-0 CAPLUS
CN 2H-Imidazo[4,5-b]quinoline-2-thione, 3-(p-ethoxyphenyl)-1,3-dihydro-9-hydroxy- (6CI) (CA INDEX NAME)



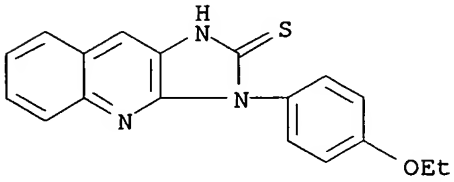
RN 113062-66-1 CAPLUS
CN 2H-Imidazo[4,5-b]quinoline-2-thione, 3-(o-ethoxyphenyl)-1,3-dihydro-9-hydroxy- (6CI) (CA INDEX NAME)



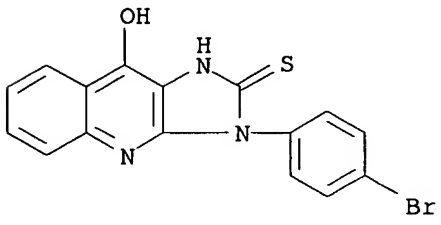
RN 113136-38-2 CAPLUS
CN 2H-Imidazo[4,5-b]quinoline-2-thione, 3-(o-ethoxyphenyl)-1,3-dihydro- (6CI) (CA INDEX NAME)



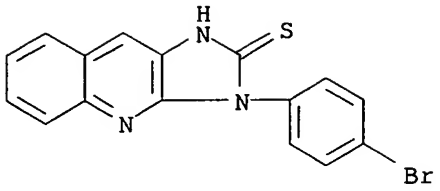
RN 113184-50-2 CAPLUS
CN 2H-Imidazo[4,5-b]quinoline-2-thione, 3-(p-ethoxyphenyl)-1,3-dihydro- (6CI) (CA INDEX NAME)



RN 131409-17-1 CAPLUS
CN 2H-Imidazo[4,5-b]quinoline-2-thione, 3-(p-bromophenyl)-1,3-dihydro-9-hydroxy- (6CI) (CA INDEX NAME)



RN 131409-44-4 CAPLUS
CN 2H-Imidazo[4,5-b]quinoline-2-thione, 3-(p-bromophenyl)-1,3-dihydro- (6CI) (CA INDEX NAME)



L25 ANSWER 421 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1961:12147 CAPLUS
DOCUMENT NUMBER: 55:12147
ORIGINAL REFERENCE NO.: 55:2326b-d
TITLE: Color developer additives
INVENTOR(S): Spath, Catherine M.
PATENT ASSIGNEE(S): Eastman Kodak Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

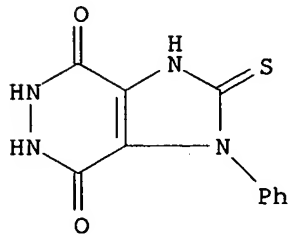
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2956876		19601018	US	
GB 898005			GB	

AB Tetraazaindene or pentaazaindene compds. containing a free SH group or its alkali metal salt will reduce fog in color materials. An additive was prepared by adding 7 g. PhNCO to a solution of 7 g. 2-hydrazino-4-hydroxy-6-methylpyrimidine in 2000 ml. hot EtOH to give 5 g. 6-hydroxy-3-mercapto-4-methyl-1,2,3a,7-tetraazaindene, m. 278°. Also prepared were 4-hydroxy-2-mercaptomethyl-6-methyl-1,3,3a,7-tetraazaindene, m. 255-9°, from 2-formamidinothiomethyl-4-hydroxy-6-methyl-1,3,3a,7-tetraazaindene; 7-amino-5-mercapto-1,2,3,4,6-pentaazaindene, m. 300°, from 2-mercapto-4,5,6-triaminopyrimidine sulfate; 3-(2-formamidoethyl)-5-mercapto-1,2,4-triazole, m. 202-3° from 3-(2-aminoethyl)-5-mercapto-1,2,4-triazole and formic acid; 5-formamido-1,3,4-triazaindene, m. 257-9°, from 2,3,6-triaminopyridine-HCl and Na formate; and tartaric bis[2-(4-hydroxy-6-methyl-2-pyrimidyl)hydrazide], m. 281-5° (decompose), from tartaric hydrazide and 2-ethylthio-4-hydroxy-6-methylpyrimidine.

IT **63886-80-6**, 1H-Imidazo[4,5-d]pyridazine-4,7-diol, 2-mercapto-1-phenyl-
(as antifoggant in color photography)

RN 63886-80-6 CAPLUS

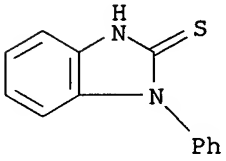
CN 1H-Imidazo[4,5-d]pyridazine-4,7-dione, 2,3,5,6-tetrahydro-1-phenyl-2-thioxo- (9CI) (CA INDEX NAME)



L25 ANSWER 422 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1960:117372 CAPLUS
DOCUMENT NUMBER: 54:117372
ORIGINAL REFERENCE NO.: 54:22307e-f
TITLE: Flotation of oxidized carbonate and silicate copper ores
INVENTOR(S): Tyurenkova, G. N.; Silina, E. I.; Postovskii, I. Ya.; Kakovskii, I. A.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 127962		19600428	SU	

AB The collector in the flotation of Cu is 1-phenyl-2-mercaptobenzimidazole. This reagent is obtained by the interaction of N-substituted o-phenylenediamine and CS2 at approx. 80°. The reaction is carried out in pyridine or pyridine bases, and the yield is 60-80%. The reagent is very effective in extracting Cu. By use of this reagent, an ore containing 1.77% Cu was extracted ≤90%.
IT **4493-32-7**, 2-Benzimidazolethiol, 1-phenyl-
(for copper ore (oxidized carbonate and silicate) flotation)
RN 4493-32-7 CAPLUS
CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



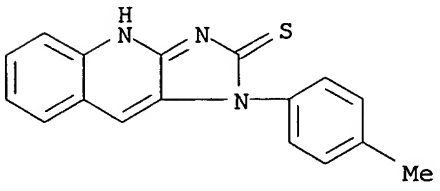
L25 ANSWER 423 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1960:50380 CAPLUS
DOCUMENT NUMBER: 54:50380
ORIGINAL REFERENCE NO.: 54:9891i,9892a-e
TITLE: Antispasmodic compounds. IV
AUTHOR(S): Sahoo, B.; Tripathy, P. B.; Rout, M. K.
CORPORATE SOURCE: Ravenshaw Coll., Cuttack
SOURCE: J. Indian Chem. Soc. (1959), 36, 421-4
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 53, 10186g. Most of the prepared compds. show musculotropic activity. RC6H4N.CO.CH2.S.C:S were prepared from ClCH2CO2Na and ammonium aryldithiocarbamates (R, % yield, and m.p. given): p-Me, 63, 159°; m-Me, 65, 149°; o-Me, 60, 105°; p-Cl, 62, 156°; m-Cl, 54, 165°. These refluxed with o-nitrobenzaldehyde in glacial HOAc and NaOAc 2.5 hrs., cooled, poured into H2O, kept overnight, filtered and washed with H2O gave the 5-(o-nitrobenzylidene) rhodanines [R, % yield, and m.p. (alc.) given]: H, 80, 240°; p-Me, 70, 180°; m-Me, 82, 176°; o-Me, 85, 170°; p-Cl, 85, 199°; m-Cl, 73, 181°. The latter were refluxed with Zn dust in HOAc until nearly colorless and worked up to the 2-thiono-3-phenyl-4,5-(2',3'-quinolino)thiazolidines [phenyl substituent, % yield, and m.p. (alc.) given]: H, 40, 110°; p-Me, 35, 122°; m-Me, 32, 255° (decomposition); o-Me, 30, 140°; p-Cl, 33, 245° (decomposition); m-Cl, 32, 110°. Anthranilic acid and N-arylrhodanine were fused at

150°; anhydrous NaOAc (fine powder) was added during 1 hr., the mass heated 5 hrs. at 135°, cooled, treated first with aqueous $NaHCO_3$ and filtered and then with cold dilute NaOH and filtered. The alkaline filtrate acidified with HCl gave 2-thiono-3-phenyl-4,5-(4'-hydroxy-2',3'-quinolino)thiazolidines [phenyl substituent, % yield, and m.p. (alc.) given]: H, 56, 280°; p-Me, 54, 280°; m-Me, 56, 300°; o-Me, 57, 250°; p-Cl, 53, 250°; m-Cl, 56, 293°. p-Tolylthiohydantoin and o-nitrobenzaldehyde refluxed in HOAc with NaOAc gave 50% 3-(p-tolyl)-5-(o-nitrobenzylidene)-2-thiohydantoin, m. 195° (alc.). The latter refluxed in HOAc with Zn dust gave 42% 2-thiono-3-p-tolyl-4,5-(2',3'-quinolino)imidazolidine, m. 223°. Anthranilic acid and 3-p-tolyl-2-thiohydantoin heated as above gave 55% 2-thiono-3-p-tolyl-4,5-(4'-hydroxy-2',3'-quinolino)imidazolidine, m. 232° (decomposition). A mixture of approx. 2 g. 4-aryl-2-aminothiazole, 1.2 g. paraformaldehyde, 1.46 g. 8-hydroxyquinoline, 2 ml. concentrated HCl, and 20 ml. alc. was refluxed 8 hrs. Excess alc. was removed; the mass solidified when kept in contact with NH_3. 4-Aryl-2-(8'-hydroxy-7'-quinolylmethylamino)thiazoles were formed [aryl group, % yield, and m.p. (alc.) given]: 4-hydroxyphenyl, 65, 152° (decomposition); 4-hydroxy-3-methoxyphenyl, 68, 135°; 1-naphthyl, 70, 128°.

IT **109728-91-8**, 2H-Imidazo[4,5-b]quinoline-2-thione, 1,3-dihydro-1-p-tolyl- **109729-13-7**, 2H-Imidazo[4,5-b]quinoline-2-thione, 1,3-dihydro-9-hydroxy-1-p-tolyl-
(preparation of)

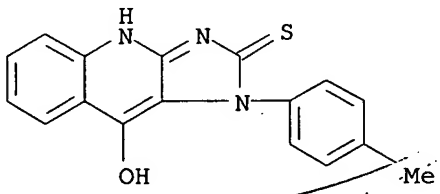
RN 109728-91-8 CAPLUS

CN 2H-Imidazo[4,5-b]quinoline-2-thione, 1,3-dihydro-1-p-tolyl- (6CI) (CA INDEX NAME)



RN 109729-13-7 CAPLUS

CN 2H-Imidazo[4,5-b]quinoline-2-thione, 1,3-dihydro-9-hydroxy-1-p-tolyl- (6CI) (CA INDEX NAME)



closest

L25 ANSWER 424 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1960:16945 CAPLUS

DOCUMENT NUMBER: 54:16945

ORIGINAL REFERENCE NO.: 54:3392b-e

TITLE: Antifungal substances. II. Syntheses and antifungal effect of mercury derivatives of 2-mercaptobenzimidazole

AUTHOR(S): Nakajima, Shotaro; Tanaka, Ichiro; Seki, Teruya; Anmo, Toshio; Komatsu, Makoto

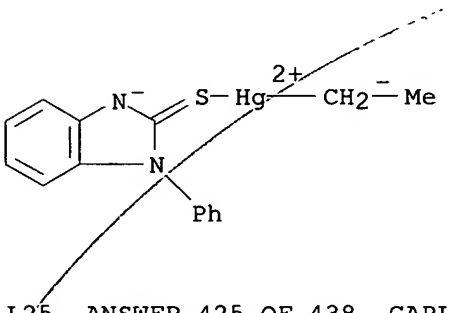
CORPORATE SOURCE: Taisho Pharm. Co., Ltd., Tokyo
SOURCE: Yakugaku Zasshi (1959), 79, 1113-16
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 53, 8124e. 2-Ethylthiobenzimidazole (I) (1.8 g.) in 20 ml 2% KOH-EtOH stirred with 2.7 g. HgBr2 in 30 ml. 2% KOH-EtOH, the KBr filtered off, the solution made up to 200 ml. with H2O, and the product filtered off gave 3.3 g. 1-EtHg derivative (II) of I, plates, m. 128-9° (70% EtOH). 1-Phenyl-2-mercaptobenzimidazole (III) (2.3 g.) in 30 ml. 2% KOH-EtOH and 3.1 g. HgBr2 in 70 ml. 2% KOH-EtOH reacted as above to give 3.5 g. 2-EtHgS analog (IV) of III needles, m. 114-15°. Similarly, 5 g. 2-mercaptobenzimidazole (V), 20 g. HgBr2, and 600 ml. 2% KOH-EtOH yielded 16 g. 1-ethylmercuri-2-(ethylmercurithio)benzimidazole (VI) needles, m. 253-4° (decomposition) (EtOH). 5(or 6)-Chloro-2-mercaptobenzimidazole (3.1 g.) in 20 ml. 10% NaOH and 8.9 g. HgBr2 in 100 ml. 10% NaOH mixed, the precipitate filtered off, washed with H2O, and the product recrystd. (EtOH) gave 10 g. 5(or 6)-chloro-1-ethylmercuri-2-(ethylmercurithio)benzimidazole (VII). V (0.8 g.) in 30 ml. 2% KOH-EtOH and 3.6 g. (PhCH2CO2)2Hg in 50 ml. 2% KOH-EtOH in a similar way yielded 3 g. 1-phenylmercuri-2-(phenylmercurithio)benzimidazole (VIII), m. above 300° (EtOH) Of these compds., II, VII, and IV inhibited the growth of Trichophyton interdigitale and T. asteroides at the dilution of 1:2,200,000, and for T. rubrum at a dilution of 1:3,300,000-5,000,000.

IT **59547-63-6**, Benzimidazole, 2-(ethylmercurithio)-1-phenyl- (preparation of)

RN 59547-63-6 CAPLUS

CN Mercury, (1,3-dihydro-1-phenyl-2H-benzimidazole-2-thionato-S)ethyl- (9CI) (CA INDEX NAME)



L25 ANSWER 425 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1960:868 CAPLUS
DOCUMENT NUMBER: 54:868
ORIGINAL REFERENCE NO.: 54:137d-i,138a
TITLE: Color developer
INVENTOR(S): Anon.
PATENT ASSIGNEE(S): Kodak Soc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 570978		19580930	BE	

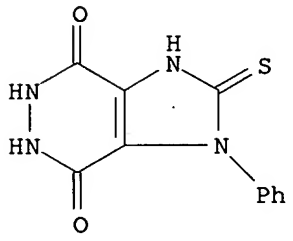
AB A new developer for reducing the colored fogging and yielding maximum color d. is of the aromatic primary amine type (substituted by OH or another NH2 group) and contains a heterocyclic compound RCH2SM or RSM with R = tetraazaindenyl or pentaazaindenyl radical and M = H or cation (Belg. 530,062). Maximum d. and fogging values are given for emulsions sensitized by polyethylene glycol oleic ester: with 4,7-dihydroxy-2-mercapto-1-phenyl-1,3,5,6-tetraazaindene (I), 3.50 and 0.10; with 4,7-dihydroxy-2-mercapto-1,3,5,6-tetraazaindene (II), 3.00 and 0.14; with 6-hydroxy-3-mercapto-4-

methyl-1,2,3a,7-tetraazaindene (III), 3.50 and 0.12; with 4-hydroxy-2-mercaptomethyl-6-methyl-1,3,3a,7-tetraazaindene (IV), 3.30 and 0.09; with 7-mercapto-1,3,4,6-tetraazaindene (V), 3.90 and 0.23; with 7-amino-5-mercapto-1,2,3,4,6-pentaazaindene (VI), 3.20 and 0.14; blank values are 3.30 and 0.31. The following compds. have also been used: 3-(2-formamidoethyl)-5-mercapto-1,2,4-triazole (VII), 5-formamido-1,3,4-triazaindene (VIII), tartaric bis[2-(4-hydroxy-6-methylpyrimid-2-yl)hydrazide] (IX), tetrachlorobenzo-1,2,3-triazole (X), α-amino-β-mercaptoisovaleric acid (XI), 2-(4-hydroxy-3-methoxyphenyl)-4-carboxythiazolidine (XII), 2-(4-hydroxyphenyl)-4-carboxythiazolidine (XIII). III is prepared by adding 7 g. phenyl isothiocyanate to a solution of 7 g. 2-hydrazino-4-hydroxy-6-methylpyrimidine in 2 l. hot EtOH and keeping reaction mixture at room temperature for 24 hrs. Crystallization from H2O yields 5 g. III, m. 278°. Treatment of 2-formamidinothiomethyl-4-hydroxy-6-methyl-1,3,3a,7-tetraazaindene in boiling dilute aqueous NaOH followed by acidification and crystallization from H2O yield IV, m. 255-9°. VI, is obtained from 16 g. 2-mercapto-4,5,6-triaminopyrimidine sulfate dissolved in 200 cc. H2O by NaOH addition; 7 g. NaNO3 is added to the filtered solution which is then acidified and heated for 1/2 hr. on steam-bath. After cooling (0°), the precipitated solid is dissolved in NaOH solution and treated with active C; after AcOH addition, solid is washed with H2O and dried; yield of VI, m. 300° is 8 g. VII is prepared by refluxing for 5 hrs. 5 g. 3-(2-aminoethyl)-5-mercapto-1,2,4-triazole in 25 cc. HCOOH 98%; evaporation to dryness under reduced pressure (steam bath), trituration of residue with a little EtOH, and recrystn. from aqueous EtOH yield 2 g. VII-hydrate, m. 202-3°. VIII, m. 257-8° is similarly obtained from 2,3,6-triaminopyridine-HCl, HCOONa and HCOOH. IX is obtained by heating, for 20 hrs. on a steam bath, a mixture of 178 g. tartaric hydrazide, 340 g. 2-ethylthio-4-hydroxy-6-methylpyrimidine in 1 l. H2O; precipitate digestion in 2 l. boiling H2O yields, after cooling, 219 g. IX, m. 281-5° (decompose) with infrared absorption at 7270 A. Preparation of XII and XIII are given in Belg. 559,754 (cf. following abstract).

IT **63886-80-6**, 1H-Imidazo[4,5-d]pyridazine-4,7-diol, 2-mercapto-1-phenyl-
(as photographic color developer)

RN 63886-80-6 CAPLUS

CN 1H-Imidazo[4,5-d]pyridazine-4,7-dione, 2,3,5,6-tetrahydro-1-phenyl-2-thioxo- (9CI) (CA INDEX NAME)



L25 ANSWER 426 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1959:45170 CAPLUS

DOCUMENT NUMBER: 53:45170

ORIGINAL REFERENCE NO.: 53:8124e-i

TITLE: Antifungal substances. I. Syntheses and antifungal effects of 2-mercaptobenzimidazole derivatives

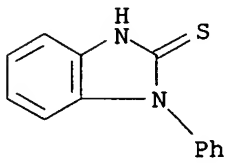
AUTHOR(S): Nakajima, Shotaro; Tanaka, Ichiro; Seki, Teruya; Anmo, Toshio

CORPORATE SOURCE: Taisho Pharm. Co., Tokyo

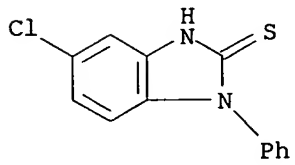
SOURCE: Yakugaku Zasshi (1958), 78, 1378-82
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB 2-Nitrodiphenylamine (64.2 g.) in 300 ml. EtOH reduced with Raney Ni and H with pressure at 40 atmospheric, the product in 150 ml. EtOH, 60 ml. H2O, 19.2 g. KOH, and 25 g. CS2 heated 4 hrs. on a H2O bath and acidified with 10% HCl gave 50 g. 1-phenyl-2-mercaptobenzimidazole (Ia), needles, m. 195° (EtOH). 2-Mercaptobenzimidazole (I) (10 g.), 10 g. KOH, 10 ml. H2O, 20 ml. EtOH and 9.2 g. BuBr stirred at room temperature, refluxed, 30 min. and the product treated with H2O gave 6.5 g. 2-butylthiobenzimidazole (II), needles, m. 134-5° (EtOH). PhSH (3 g.) in 30 ml. EtOH and 1.4 g. KOH refluxed 3 hrs. with 4 g. 2-chlorobenzimidazole, the KCl filtered off and the filtrate cooled gave 2 g. 2-phenylthiobenzimidazole, needles, m. 201° (EtOH). 2-(2-Hydroxyethylthio)benzimidazole (III) (4 g.) and 10 g. SOCl2 heated 30 min. on a H2O bath, the product concentrated, the residue poured into ice H2O and made alkaline with K2CO3 gave 2 g. 2-(ClCH2CH2S) analog of III, m. 122-4° (EtOH). I (10 g.) and 10 g. Me2NCH2CH2Cl.HCl in 50 ml. AmOH refluxed 5 hrs., cooled, the precipitate filtered off, washed with Et2O, taken up in 10% Na2CO3 and the solution made alkaline gave 10.5 g. 2-(Me2NCH2CH2S) analog of I, needles, m. 145-6° (EtOH). Catalytic reduction of 3 g. 2-(2-dimethylaminoethylthio)-5-nitrobenzimidazole (IV) in 50 ml. EtOH with Raney Ni yielded 1 g. 5-NH2 analog of IV, m. 85-6° (C6H6). Ia (7.5 g.) in 25 ml. C5H5N treated dropwise with BzCl, stirred 2 hrs., and the product poured in H2O gave 1.8 g. 2-BzS analog of Ia, needles, m. 160-3° (EtOH). Of 59 derivs. of I tested for growth inhibition of Trichophyton interdigitale, II and the 2-iso-BuS and 5-Cl-2-PhCH2S analogs of I were effective at a dilution above 1:291,900.

IT **4493-32-7**, 2-Benzimidazolethiol, 1-phenyl-
(esters)
RN 4493-32-7 CAPLUS
CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



IT **96459-92-6**, 2-Benzimidazolethiol, 5-chloro-1-phenyl-
(preparation of)
RN 96459-92-6 CAPLUS
CN 2-Benzimidazolethiol, 5-chloro-1-phenyl- (6CI, 7CI) (CA INDEX NAME)



L25 ANSWER 427 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1958:104328 CAPLUS

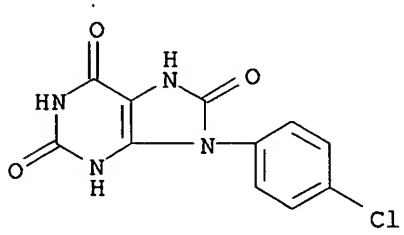
DOCUMENT NUMBER: 52:104328
ORIGINAL REFERENCE NO.: 52:18426h-i,18427a-i,18428a-b
TITLE: Potential purine antagonists. XI. Synthesis of some 9-aryl(alkyl)-2,6-disubstituted purines
AUTHOR(S): Koppel, Henry C.; Robins, Roland K.
CORPORATE SOURCE: Arizona State Coll., Tempe
SOURCE: Journal of the American Chemical Society (1958), 80, 2751-5
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 52:104328
AB cf. C.A. 52, 13741h. NaNO2 (40 g.) added to 100 g. barbituric acid in 1 l. H2O at 70-80°, allowed to stand 10 min., treated with stirring with 200 g. Na2S2O4 in portions below 90°, cooled to room temperature, and filtered yielded 92 g. 5-amino-2,4,6-trihydroxypyrimidine (uramil) (I). I (70 g.) in 1500 cc. N NaOH treated at 60° with stirring dropwise with 66 g. PhNCS during about 1.5 hrs., stirred 2 hrs. at 60°, acidified with glacial AcOH, cooled, and filtered yielded 95 g. N-(2,4,6-trihydroxy-5-pyrimidyl)-N'-phenylthiourea, plates, m. above 300°. 2,6-Dihydroxy-9-phenyl-8-purinethiol (50 g.) in 500 cc. N NaOH refluxed 3 hrs. with 150 g. wet Raney Ni, filtered, cooled to 4°, and filtered again, the filtrate refluxed again 3 hrs. with 150 g. fresh Raney Ni and processed as before, the combined filter residues dissolved in boiling H2O, and the solution treated with C and acidified with concentrated HCl gave 20 g. 2,6-dihydroxy-9-phenylpurine (II), plates, m. above 300°. II (8 g.) and 24 g. P2S5 ground together, diluted with 500 cc. dry pyridine, refluxed 3 hrs., the excess pyridine removed in vacuo, the residue diluted with 500 cc. iced H2O, the solution kept at room temperature, refluxed 2 hrs., acidified with HCl, cooled, and the crude product (4.5 g.) repptd. twice from hot dilute aqueous KOH gave 2-hydroxy-9-phenyl-6-purinethiol-H2O, light yellow needles, m. above 300°; it lost 1 mole H2O at 180°. II (20 g.), 500 cc. POCl3, and 100 g. PCl5 refluxed 40 hrs., the excess POCl3 removed in vacuo, the residue poured with stirring onto crushed ice, the solution extracted with six 1-l. portions Et2O, and the extract worked up gave 12 g. 2,6-dichloro-9-phenylpurine (III), pale yellow needles, m. 244-6° (EtOAc); the insol. residue (3.0 g.) from the Et2O extraction boiled in N NaOH gave 1.2 g. 2-chloro-6-hydroxy-9-phenylpurine (IV). III (3 g.) refluxed 3 hrs. in N NaOH, the solution treated with C, filtered, chilled, the precipitate filtered off, washed, dissolved in boiling H2O, and the solution acidified with glacial AcOH while hot gave 1.9 g. IV, needles, m. 280-1° (EtOH). III (5 g.) added to 200 cc. absolute MeOH containing 10 g. CS-(NH2)2, refluxed 6 hrs., and cooled yielded 3 g. 9-phenyl-2,-6-purinedithiol, light green needles, m. above 300° (90% EtOH). III (5 g.) in 100 cc. EtOH heated on the steam bath with 12 cc. PrNH2 to solution and then an addnl. 3 hrs. and cooled gave 4.0 g. 2-chloro-6-propylamino-9-phenylpurine, needles, m. 121-2° (decomposition) (80% EtOH). III (4 g.) added to 75 cc. absolute EtOH containing 1.9 g. Ph(CH2)2NH2, heated 1.5 hrs. on the steam bath, treated with C, filtered, cooled, and treated 20 min. with a stream of dry HCl gave 5.4 g. 2-chloro-6(2-phenylethylamino)-9-phenylpurine-HCl (V.HCl), m. 172-4° (absolute EtOH). III (5 g.) in 70 cc. H2O heated 8 hrs. on the steam bath with 20 cc. 40% aqueous Me2NH, cooled, and filtered gave 3.5 g. 6-(Me2N) analog of V, needles, m. 168-9° (EtOH). N-(2,4,6-Trihydroxy-5-pyrimidyl)-N'-(p-chlorophenyl)thiourea (40 g.) refluxed 5 hrs. in 650 cc. concentrated HCl, diluted to 1 l. with H2O, and filtered immediately gave 23 g. 2,6-dihydroxy-9-(p-chlorophenyl)-8-purinethiol (VI), light yellow, m. above 300° (aqueous AcOH). VI (30 g.) in 500 cc. N NaOH refluxed 3 hrs. with 90 g. wet Raney Ni, filtered, cooled to 10°, and filtered again yielded 9.0 g. Na salt of the p-Cl deriv, of II. 2,6-Dihydroxy-9-methyl-8-purinethiol (VII) (10 g.) treated similarly with Raney Ni and the resulting Na salt acidified with

glacial AcOH gave 4.8 g. 2,6-dihydroxy-9-methylpurine (VIII), m. above 300°. The 9-Et homolog of VII (17.0 g.) gave similarly 6 g. 9-Et homolog of VIII. N-(2,4,6-Trihydroxy-5-pyrimidyl)-N'isobutylthiourea (25 g.) refluxed 5 hrs. in 250 cc. concentrated HCl, diluted to 500 cc. with H2O, and filtered immediately yielded 16 g. 9-iso-Bu analog (IX) of VI. IX (10 g.) in 200 cc. N NaOH refluxed 3 hrs. with 30 g. Raney Ni yielded 5.0 g. 9-iso-Bu homolog of VIII. 2-Amino-4,6-dihydroxypyrimidine (100 g.) in 800 cc. 0.5N NaOH treated at 60° with 40 g. NaNO2 and then with concentrated HCl, filtered, the residue washed with a little H2O, suspended in 1 l. H2O at 20°, treated carefully with 25 g. Na2S2O4, boiled 5 min., and filtered hot, and the deposit from the filtrate recrystd. from H2O gave 38 g. 2,5-diamino-4,6-dihydroxypyrimidine (X). X (25 g.) in 400 cc. N NaOH treated at 60-70° with 13 g. MeNCS, stirred 4 hrs., acidified with glacial AcOH, kept 6 hrs. at room temperature, and filtered yielded 25 g. N-(2-amino-4,6-dihydroxy-5-pyrimidyl)-N'-methylurea (XI); it became highly colored in air. Crude XI (25 g.) and 250 cc. concentrated HCl refluxed 5 hrs., diluted to 450 cc. with H2O, and filtered immediately gave 14 g. crude 2-amino-6-hydroxy-9-methyl-8-purinethiol, which refluxed successively in the usual manner with two 42-g. portions wet Raney Ni in 250 cc. N NaOH yielded 7.5 g. 2-amino-6-hydroxy-9-methylpurine (XII), m. above 300° (aqueous HCONMe2). X (23 g.) treated in the usual manner with 20 g. iso-BuNCS and the resulting N-(2-amino-4,6-dihydroxy-5-pyrimidyl)-N'-isobutylurea cyclized in HCl gave 12 g. crude product which desulfurized in the usual manner with two 40-g. portions wet Raney Ni in 250 cc. N NaOH gave 5.1 g. 9-iso-Bu homolog of XII. X (25 g.) treated with 17 g. EtNCS, the resulting product cyclized with concentrated HCl, and the 2-amino-6-hydroxy-9-ethyl-8-purinethiol (14 g.) desulfurized with Raney Ni in the usual manner gave 6.0 g. 9-Et homolog of XII. XII (8 g.) and 32 g. P2S5 in 500 cc. dry pyridine refluxed 8 hrs., the pyridine removed in vacuo, the residue treated with 500 cc. iced H2O, the solution heated 3 hrs. on the steam bath and chilled overnight, and the crude deposit (5.0 g.) precipitated twice from hot, dilute aqueous NaOH with AcOH gave 2-amino-9-methyl-6-purinethiol, light yellow, m. above 300°. I (71 g.) in 1.5 l. N NaOH treated at 60-70° dropwise with stirring with 75 g. p-ClC6H4NCO during about 1.5 hrs., stirred 2 hrs. at 60-70°, cooled, acidified with glacial AcOH filtered, the residue washed with a little H2O and refluxed 6 hrs. with 1 l. concentrated HCl, diluted with H2O to 1500 cc., and the precipitate washed with H2O and dried gave 70 g. 9-(p-chlorophenyl)uric acid (XIII), needles, m. above 300° (AcOH). I (54 g.) and 50 g. o-ClC6H4NCO gave similarly 49.0 g. o-isomer of XIII, needles, m. above 300° (aqueous AcOH). The ultraviolet absorption maximum of the substituted purines reported are tabulated.

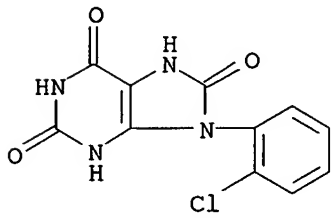
IT **5444-39-3**, Uric acid, 9-[p-chlorophenyl]- **5444-40-6**, Uric acid, 9-[o-chlorophenyl]- **115164-08-4**, Uric acid, 9-(p-chlorophenyl)-8-thio-
(preparation of)

RN 5444-39-3 CAPLUS

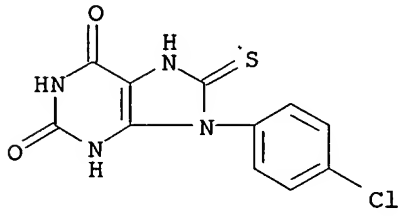
CN 1H-Purine-2,6,8(3H)-trione, 9-(4-chlorophenyl)-7,9-dihydro- (9CI) (CA INDEX NAME)



RN 5444-40-6 CAPLUS
CN 1H-Purine-2,6,8(3H)-trione, 9-(2-chlorophenyl)-7,9-dihydro- (9CI) (CA INDEX NAME)



RN 115164-08-4 CAPLUS
CN Uric acid, 9-(p-chlorophenyl)-8-thio- (6CI) (CA INDEX NAME)



L25 ANSWER 428 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1958:77210 CAPLUS
DOCUMENT NUMBER: 52:77210
ORIGINAL REFERENCE NO.: 52:13712b-i,13713a-g
TITLE: Synthesis of some substituted benzimidazolinones
AUTHOR(S): Clark, Robert L.; Pessolano, Arsenio A.
CORPORATE SOURCE: Merck, Sharp & Dohme Research Labs., Rahway, NJ
SOURCE: Journal of the American Chemical Society (1958), 80, 1657-62
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 52:77210

AB The appropriate aromatic o-diamine in aqueous HCl treated with COCl2 until the precipitate formation was complete, filtered, and the precipitate with H2O gave the corresponding substituted 2-benzimidazolinone (I) (substituents and m.p. given): 4-Me, 302-3° (MeOH); 4,7-di-Me, 337° (AcOH); 5-Et, 264-5° (EtOH); 4-Et, 261-2° (EtOH); 5-Pr, 239-41° (aqueous EtOH); 5-iso-Pr, 270-2° (EtOH); 5-Bu, 250° (aqueous EtOH); 5-EtMeCH, 253-4° (aqueous EtOH); 5-Me3C, 310° (aqueous EtOH); 5-EtMe2C, 284-5° (aqueous EtOH); 5-MePrCH, 217-18° (EtOAc); 5-C6H13, 250-2° (EtOAc); 5-Ac, 296-7° (aqueous EtOH); 5-HO, 307-9° (aqueous EtOH); 5-MeO, 256-7° (EtOH); 5-F, 303° (aqueous EtOH); 4-iso-Pr, 7-Br, 245-9° (aqueous EtOH); 5-Br, 336-7° (AcOH); 4-Cl, 335-6° (aqueous EtOH); 1-Et, 5-Me, 115° (aqueous EtOH); 1-Ph, 206-7° (EtOH); 1,5-di-Me, 197-9° (aqueous EtOH); 1-Et, 117-18° (Et2O-petr. ether); 4,5-CH:CHCH:CH, above 345° (HCONMe2-Et2O). The appropriate aromatic o-diamine (1.0 mole) (or its HCl salt) and 1.1 moles urea heated at 140° or higher during 15 min., cooled, dissolved in 2.5N NaOH, filtered, acidified with concentrated HCl, and the base-acid treatment repeated or the precipitate recrystd. gave the corresponding

I (same data given): 5,6-di-Me, above 345° (AcOH); 5-Ph, 350° (AcOH); 5,6-di-MeO, 268° (dioxane); 4,6-di-Cl, above 340° (aqueous dioxane); 5,6-di-Cl, 345° (repptd.); 4,5,6-tri-Cl, 342° (repptd.). The appropriate nitro compound in EtOH hydrogenated at 40 lb. over 5% Pd-C, filtered, and evaporated (or treated with dry HCl) gave the corresponding amino analog (m.p. given): 5-amino-1,3-dimethylbenzimidazolone-0.5-H2O.HCl, 310° (MeOH-Et2O); 5-aminobenzimidazolone-HCl, above 340° (EtOH-Et2O). The following substituted o-phenylenediamines (substituent and m.p. given): 4-Et.2HCl, 308° (EtOH-Et2O); 3-Et.HCl, 258° (EtOH); 4-Pr.2HCl, 206-10° (EtOH-Et2O); 4-iso-Pr.2HCl, 267° (aqueous EtOH); 4-Bu.2HCl, 235° (EtOH); 4-EtMeCH.2HCl, 249-51° (EtOH-Et2O); 4-MePrCH.2HCl, 214-17° (EtOH); 4-Ac.HCl, 280-7° (aqueous EtOH); 4-MeO.2HCl, 227° (EtOH-Et2O); 4,5-di-MeO.HCl, 230-50° (aqueous MeOH); 4,2-Me(H2N)C6H3NHEt.2HCl, 178-80° (EtOH); o-H2NC6H4NHEt.HCl, 188-93° (EtOH-Et2O). SnCl2.2H2O (100 g.) in 180 cc. concentrated HCl treated portionwise with stirring with 30 g. 4,2-Ph(O2N)C6H3NH2 below 40°, stirred 2 hrs., kept at room temperature overnight, added below 10° to 350 g. NaOH in about 800 cc. cold H2O, filtered after 3 hrs., and the residue repptd. from 700 cc. hot EtOH with H2O gave 20 g. 3,4-(H2N)2C6H3Ph, m. 102-3°. 4,2-iso-Pr(O2N)C6H3NHAc (17.5 g.) in 125 cc. concentrated HCl heated 3 hrs. on the steam bath, cooled to 50°, treated slowly with stirring with 75 g. SnCl2.2H2O in 30 cc. H2O and 15 cc. concentrated HCl, cooled to room temperature, treated with C, filtered, and treated directly with COCl2 gave 5-isopropylbenzimidazolinone. The appropriate benzimidazolinone refluxed 3 hrs. with 5 parts acid anhydride and cooled gave the corresponding I (substituents and m.p. given): 1-Me, 3-Ac, 120-1° (EtOH); 1-Ph, 3-Ac, 137-8° (EtOH); 1,3-di-Ac, 5-AcNH, 260-1° (aqueous AcOH; 1,3-di-Ac, 5-Me3C, 127-30° (EtOAc-petr. ether); 1,3-di-EtCO, 169-70° (EtOAc); 1,3-di-Ac, 5-Cl, 172-3° (EtOAc); 1,3-di-Ac, 5-NO2, 131-2° (EtOH); 1,3-di-Ac, 5,6-di-Cl, 218-19° (dioxane); 1-Ac, 3-Me, 120-1° (EtOH); 1-Me, 3-AcOCH2, 115-16° (EtOAc). Benzimidazolinone (152 g.) and 365 g. powdered KOH in 2000 cc. Me2CO refluxed with stirring, the mixture treated dropwise with 432 g. MeI in 350 cc. Me2CO, heated 10 min., decanted, the pasty residue extracted 3 times with Me2CO, the extract evaporated, and the crystalline material recrystd. from 450 cc. hot C6H6 by the slow addition of 100 cc. petr. ether gave 122 g. 1,3-dimethylbenzimidazolinone, m. 111-12°; 39 g. 2nd crop. Similarly were prepared the following I (same data given): 1,3-di-(CH2CH:CH2), 53-4° (petr. ether); 1,3-di-(PhCH2), 107-8° (Et2O); 1,3-di-Me, 5-Me3C, 180-1° (aqueous EtOH); 1,3-di-Me, 5-iso-Pr, 142-3° (aqueous EtOH); 1,3-di-(CH2CMe:CH2), 85-6° (Et2O-petr. ether); 1,3,5,6-tetra-Me, 153-4° (EtOAc); 1,3-di-Me, 5-Cl, 163-41° (aqueous EtOH); 1,3,5-tri-Me, 103-5° (Et2O-petr. ether); 1,3-di-Me, 5-MeO, 92-3° (C6H6-petr. ether); 1,3-di-Et, 68-9° (petr. ether); 1,3-di-(PhCH2CH2), 74-5° (Et2O-petr. ether); 1,3-di-Me, 5-Br, 166-7° (EtOH); 1,3-di-Me, 5-EtO, 104-5° (aqueous EtOH); 1,3-di-(BzCH2), 197-8° (aqueous AcOH); 1,3-di-(Me2NCH2CH2).2HClO4, 238° (aqueous EtOH); 1,3-di-(EtO2CCH2), 169-70° (EtOH); 1,3-di-(Et2NCH2CH2), 5-Me3C.2HClO4, 140° (aqueous EtOH); 1,3-di-(Et2NCH2CH2).2HClO4, 142-3° (MeOH); 1,3-di(Et2NCH2CH2), 4,6-di-Me.2HClO4, 201-3° (aqueous EtOH); 1,3-di-(Me2NCHMeCH2.).2HClO4, 229-30° (aqueous EtOH); 1,3-di-(Et2NCH2CH2), 5-MeO.2HClO4, 160-2°; 1,3-di-Me, 5-NO2, 208-9° (EtOAc); 1,3-di-Me, 5-H2NCONH, 350° (aqueous AcOH). The following I (substituents and m.p. given) were prepared by the method of Vaughan and Blodinger (C.A. 50, 8606g): 5-BuCO, 269-71° (aqueous EtOH); 5-iso-BuCO, 268-70° (EtOH); 5-C7H15CO, 246-7° (EtOH); 5-C13H27CO, 229° (EtOH). 5-Myristoylbenzimidazolinone (100 g.) in 1500 cc. EtOH hydrogenated 3.5 hrs. at 225° over 10 g. Cu chromite,

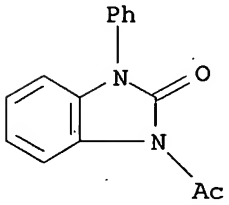
filtered, extracted with hot dioxane, and the filtered extract cooled gave 65 g.

5-tetradecylbenzimidazolinone, m. 226° with previous softening (AcOH). Similarly were prepared the following I (substituent and m.p. given): 5-Am, 261-4° (aqueous EtOH); 5-iso-Am, 256-9° (aqueous EtOH); 5-C8H17, 240-2° (EtOH). p-AcNHC6H3Ac (47 g.) in 150 cc. AcOH and 50 cc. Ac2O treated with stirring with 23 cc. fuming HNO3 at 40°, stirred 1 hr., poured into 1500 cc. H2O, and the gummy precipitate (45 g.) crystallized from 115 cc. AcOH gave 20 g. 4,3-AcNH(O2N)C6H3Ac, m. 140-1°. In the same manner were prepared the following substituted benzenes (m.p. given): 4,2-Pr(O2N)C6H3NHAc, 135° (aqueous EtOH); 3,2-iso-Pr(O2N)C6H3NHAc, 81-2° (aqueous EtOH); 4,2-EtMe2C(O2N)C6H3NHAc, 53-4° (petr. ether); 4,2-C6H13(O2N)C6H3NHAc, 51-2° (aqueous EtOH); 4,2-F(O2N)C6H3NHAc, 72-3° (aqueous EtOH); 4,5,2-Br(iso-Pr)(O2N)C6H2NHAc, 139-41°. p-MePrCHC6H4NH2 acetylated in the usual manner gave the N-Ac derivative, m. 122-4° (Et2O-petr. ether). Similarly was prepared p-C6H13C6H4NHAc, m. 74-6° (petr. ether). The appropriate acylamine heated 3 hrs. with HCl or with NaOMe by the method of Verkade and Witjens (C.A. 38, 23228) gave the corresponding amine; in this manner was prepared 4,2-Pr(O2N) C6H3NH2, m. 59-60° (aqueous EtOH). By catalytic hydrogenation of the corresponding 6-Br compound was prepared the 5-iso-Pr derivative, m. 232-3° (aqueous EtOH), of benzimidazolinone (II). The 5-NH2 derivative of II in acid treated with KOCN gave the 5-NHCONH2 derivative of II, m. 345° (repptd.). II, EtCOCl, and PhNO2 refluxed 4 hrs. gave the 1-EtCO derivative of II, m. 212-13° (EtOH). 1-Me derivative of II refluxed with aqueous CH2O gave the 3-CH2OH derivative, m. 153-4° (EtOH). The 5-Me3C derivative of II was converted by the method of Monti (C.A. 38, 45991 to the 1-xanthyl derivative, m. 253-4° (EtOAc). 1,3-Di-(HO2CCH2) derivative of II, m. 291-2° (EtOH), was prepared by hydrolysis of the di-Et ester. 5,6-Di-NO2 derivative of II reduced and the resulting diamine treated with COCl2 gave the 5,6-(NHCONH) derivative of II.0.5H2O, m. above 340° (EtOH).

IT **78162-50-2**, 2-Benzimidazolinone, 1-acetyl-3-phenyl- (preparation of)

RN 78162-50-2 CAPLUS

CN 2H-Benzimidazol-2-one, 1-acetyl-1,3-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



L25 ANSWER 429 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1957:43354 CAPLUS

DOCUMENT NUMBER: 51:43354

ORIGINAL REFERENCE NO.: 51:8096e-i,8097a-i,8098a-f

TITLE: Pseudo bases. I. Additions of methyl and methylene ketones to pyridinium salts

AUTHOR(S): Krohnke, Fritz; Ellegast, Konrad; Bertram, Ewald

CORPORATE SOURCE: Forschungsinst. Dr. A. Wander, A.-G., Sackingen/Baden, Germany

SOURCE: Ann. (1956), 600, 176-98

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB Pyridinium, quinolinium, and isoquinolinium bases form addition compds. with simple Me ketones and with certain methylene ketones. The adducts are easily retrograded by acids, and can be dehydrogenated to form bases that yield stable salts. The adducts are considered to be "salts" in which the organic cation and anion are stabilized with regard to resonance, and which are related to bases (termed mesomeric cations) which are considered intermediate between ammonium arid carbinol bases. The possibility of existence. of pseudo bases (i.e. carbinol bases) increases with decreasing aromaticity of the heterocycle. With hyperaromatic N-heterocycles like pyridine, such bases could not be isolated. In the case of quinoline and isoquinoline derivs., in certain instances such bases could be prepared, but the formation of mesomeric cations was favored. In the acridine series, and with heterocycles containing O, carbinol bases are favored over ammonium or mesomeric cations; this also occurs in the Ph3CH series. Hydrogenation of heterecycles greatly increases the stability of the carbinol bases, which are easily isolated. 2,6-Cl2C2H2Me (322 g.) in 400 cc. CCl4, stirred and irradiated was treated dropwise with 100.2 cc. Br in 50 cc. CCl4 giving 422 g. 2,6-Cl4C4H4CH4Br (I), m. 55°; details of purification are given. I is a powerful lacrimator. I with a slight excess of pyridine (cf. C.A. 47, 1704f), heated in Me2CO gave, in excellent yield, N-(2,6dichlorobenzyl)pyridinium bromide (II) m. 216-17°; this in MeOH with p-ONC6H4NMe6 (IIa) gave 58% 2,6-Cl6C6H6CH:N→O) C6H6NMe6-4 (III), yellow prismatic spikes, m. 152-3°. When 10% pyridine or α-picoline was added to the MeOH, 75% and 81% III, resp., were obtained. Formed similarly from I and appropriately substituted pyridines were the following derivs. of II: 93% 3-Me, m. 183-4° (from 1:1 EtOH-Et2O); 89% 3-HOCH2.H2O, m. 111-13°; 97% 3-H2NCO (IIIa), m. 246-8°; 95% 3-Et2-NCO, m. 197°; 90% 3-NC, m. 187-8°; and 96% 3-AcNH, m. 231°. II (1.92 g.) in 15 cc. Me2CO and 3 cc. H2O at 20° with 5 cc. 2N NaOH gave 1.69 g. Me2CO adduct, C2H2ONCl2 (IV), colorless rhombs, m. 94-5° (when cooled to 0°; not recrystallizable), forming a brown resin on standing. Similarly formed were the following adducts of II, analogs of IV; 58% BzMe (IVa), pale yellow prisms, m. 80-1°; 70% cyclohexanone, yellowish leaflets, m. 83-4°; 66% deoxybenzoin, yellow, m. 87-8°; and 79% monohydrate of the 3-H2NCO derivative of IV, m. 138-9° (decomposition). In the following dehydro compds. R: = N-[2,6-dichlorobenzyl]-1,4-dihydro-4-pyridylidene. To 6.38 g. II in 25 cc. MeOH, 5 cc. BzMe, and 1.8 g. IIa at 20° under N was added 20 cc. 2N NaOH, giving, after 4 hrs. 5.4 g. R:CHBz (IVb), dark yellow rhombs, m. 166-7° (HClO4 salt, leaflets, m. 216-17°; HBr salt, thin rhombs, m. 187-88°). Similarly formed were the following compds. (reaction time in hrs., % yield, crystalline color and form, and m.p. given): R: CHAc (IVc), 3, 97, yellow needles changing to octahedra, 203-4° (HClO4 salt colorless, m. 192-3°); R:CHCOEt, 1.5, 19, yellow prisms, 219-20°; R:CHCOC6H4Me-4, 7, 70, yellow needles, 213-14°; R:CHCOC6H4OMe-4, 21, 72.6, yellow needles, 199-200°; R:CHCOC6H4Br-4, 7, 59.8, yellow prisms, 218-19°; R:C. CH2.CH2.CH2.CO, 4, 60, yellow rectangles with violet luster, 229-30°; R: C.CO.CH2.CH2.CH2.CH2, 2, 98.5, yellow prisms, 209-10°; R: C. CO. CH2.CHMe.CH2.CH2, 2.5, 90, orange polyhedrons, 207-8° (resinifying on storage); R:C.CO.CH2.CH2.CHMe.CH2, 2, 77.8, yellow triboelectric needles, 186°; R:C.CH2.CH2.CH2.CH2.CH2.CO, 20, 46, yellow prisms, 167-8°; R: CH-NO2, 2, 14.8, yellowish brown leaflets with blue luster, 233-5° (sintering at 230°). The following were prepared using aeration (instead of IIa) and 2N MeONa in place of aqueous NaOH: R:C(CN)2, 24, 30, colorless needles, 234-5°; cyclopentadienylidene analog, 40, 51°, red prisms with blue luster, 199-20° (from HCONMe2); 1-indenylidene analog (V), 30, 23, red microprisms with steely luster, 234-5° (from C6H6). The 9-fluorenylidene analog of V, C25H17NCl2, dark red prisms with blue luster, m. 232-3°, when formed with IIa, 55.7% yield in 90 hrs., with air, 10% in 96 hrs. Using air as oxidant, 0.64 g. II, 0.3 g.

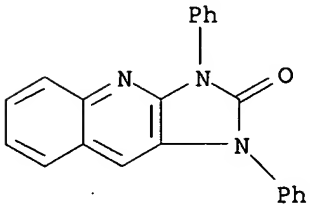
1,3-indandione in 10 cc. MeOH containing 0.4 cc. 10N NaOH gave, after 24 hrs., 0.32 g. N-[2,6-dichlorobenzyl]-4-[1,3-dioxo-2-hydrindylidene]-1,4-dihydropyridine, C12H13O2NCl2, yellow, m. 334-5° (from AcOH). Similarly, II and 1-phenyl-3-methyl-5-pyrazolone gave 70% N-[2,6-dichlorobenzyl]-4-[1-phenyl-3-methyl-5-pyrazolon-4-ylidene]-1,4-dihydropyridine, yellow, m. 223-4°. The following compds., R'N.CH:CH2C(:CHR'').CR''':-CH, formed by dehydrogenation (with IIa) of the appropriate ketone adducts (R' = 2,6-Cl2C6H3CH2; R''',R'', reaction time, % yield, crystalline properties, and m.ps. given): Me, Ac, 3, 89, yellow rhombs, 193° (HClO4 salt, m. 190-1°; HBr salt, hexagons, m. 216-18°); CH2OH, Ac, 1.5, 95.6, yellow hexagons, 205-6°; CH2OH, Bz, 17, 65, yellow rhombs, 207° (decomposition) (HBr salt, yellow, m. 220-1°, yellowish green ultraviolet fluorescence); CONH2 Ac, 1.5, 97.6, yellow, 220-1° (HBr salt, decompose 289°); CONH2, Bz, 3, 89, -, -(HCl salt, yellow rhombic leaflets, 271-2°); CONH2, p-MeOC6H4CO, 72, 85, yellow, 278-9° (HCl salt, orange prisms, 271-2°, blue ultraviolet fluorescence in H2O); CONEt2, Bz, 7.97, yellow, 201°; CONEt2 Ac, 5.5, 86.5, yellow hexagons, 170-1° (when crude, m.p. lower on recrystn.); CONH2, (:CHR'' =) 2-cyclohexanonylidene, 7, 71.4, yellow rectangles, m. 201-2° (decomposition). The 3,4-Cl2 isomer of II (0.96 g.) in 10 cc. Me2CO and 10 cc. H2O at 20° was shaken with 0.6 cc. 10N NaOH, 20 cc. Me2CO added to dissolve the resin, and then 0.63 g. KMnO4 in 10 cc. Me2CO. The warmed mixture was filtered, treated with C, refiltered, H2O added to incipient cloudiness and cooled to 0° giving 0.32 g. N-[3,4-dichlorobenzyl]-4-acetonylidene-1,4-dihydropyridine (VI), yellow, m. 146-7° (from 1:1 C6H6-ligroine). Similarly formed were the 2,4-dichloro isomer of VI, yellow, m. 144-5° and the 4-monochloro analog of VI, yellow, m. 133-4° (from Et2O). VI and its isomer and analog resinify on standing. Oxidation of IVa in pyridine, with KMnO4 gave IVb. Formed similarly was the 3,4-dichloro isomer of IVb, yellow, m. 166° (cf. Baker and McEvoy, C.A. 50, 3454g). In place of IIa, K nitrosodisulfonate converted IV into 77% IVc. IV (0.62 g.) in dry C6H6 with 0.22 g. benzoquinone in 20 min. formed 0.75 g. adduct IVc.1,4-C6H4(OH)2, orange prisms, m. 176-8°, also formed from IVc and 1,4-C6H4(OH)2, readily reconverted into IVc by treatment with HClO4 followed by treatment with 2N NaOH. In the following cases adducts of N-phenethylpyridinium bromide (VII) were not isolated but dehydrogenated directly. E.g., 2.64 g. VII with 0.8 g. IIa and 3 cc. BzMe in 15 cc. MeOH under N, with 2 cc. 10N NaOH gave 1,6 g. N-phenethyl-4-phenylidene-1,4-dihydropyridine, yellow hexagons, m. 198-9° (from 50% MeOH, the mother liquor from which gave 0.05 g. azoxydimethylaniline, orange, m. 241-2°). Similarly prepared from Me2CO was the 4-acetonylidene analog, yellow rectangles, m. 187-8°. Formed from the appropriate pyridinium salts, sometimes under slightly modified conditions were the following 4-acetonylidene-1,4-dihydropyridines: 45% N-PhCH(OH)CH2, yellow rhombs, decompose about 227-8°; 72% N-[4-ClC6H4CH2CH2], yellow leaflets, m. 193-4°; 34.3% N-[4-ClC6H4CH(OH)CH2], yellow rhombs, m. 230-1° (decomposition); 42% N-[4-O2NC6H4CH(OH)CH2], slender yellow leaflets, decompose 220°; N-[β-2-chlorostyryl], reddish brown leaflets, m. 182-3° (from C6H6). Similarly formed were the following 4-phenacylidene-1,4-dihydropyridines: N-PhCH(OH)CH2, yellow leaflets, decompose 227-8°; N-[β-4-chlorostyryl], nacreous, orange leaflets, m. 230° (decomposition); N-(β-styryl), orange leaflets, m. 208-9° (sintering 188°); N-[β-2-chlorostyryl), reddish orange hexagons, m. 212°. The following 1,4-dihydropyridines; were also formed using air and NaOH in MeOH: 90% N-(β-styryl)-4-(1-phenyl-3-methyl-5-pyrazolon-4-ylidene), red slender leaflets, m. 239-40° and 43% N-(β2-chlorostyryl)-4-(2-cyclohexanonylidene), yellowish brown leaflets, m. 192-3°. Nicotinamide MeBr salt (2.17 g.) (VIII), 3 cc. BzMe, 0.8 g. IIa, and 60 cc. MeOH under N with 2 cc. 10N NaOH gave 1 g. N-methyl-4-phenacylidene-1,4-dihydronicotinamide (IX), yellow leaflets, m. 278-9° (decomposition), which with HBr at 100° formed

2-methyl-5,8-dihydro-5-phenyl-8-oxo-2,7-naphthyridinium bromide, yellow prisms, decompose 299-300°. VIII with 4-MeOC6H4Ac gave 35.2% 4-MeO derivative of IX, brownish yellow, nacreous leaflets, decompose 277-8°; HBr salt-H2O, yellow needles, m. 278-9° (decomposition). N-(Diphenylmethyl)-4-(1-phenyl-3-methyl-5-pyrazolon-4-ylidene)-1,4-dihydropyridine, yellow, prisms, m. 238-9°. IVc (0.882 g.) in 50 cc. EtOH with 0.2 g. MgO was shaken at 20° with 50 mg. Pt black and hydrogenated. After filtration, and washing the residue with EtOH, the evaporated filtrates gave an oil which with 5 cc. N HClO4 gave 1.15 g. N-(2,6-dichlorobenzyl)-4-acetonylpiperidine-HClO4, colorless, m. 167-8° (from Me2CO). 39 references.

IT **116600-20-5**, 2H-Imidazo[4,5-b]quinolin-2-one, 1,3-dihydro-1,3-diphenyl-
(preparation of)

RN 116600-20-5 CAPLUS

CN 2H-Imidazo[4,5-b]quinolin-2-one, 1,3-dihydro-1,3-diphenyl- (6CI) (CA INDEX NAME)



L25 ANSWER 430 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1957:43353 CAPLUS

DOCUMENT NUMBER: 51:43353

ORIGINAL REFERENCE NO.: 51:8096b-e

TITLE: N-Substituted 2,3-diaminopyridines and 2,3-dianilinoquinoline

AUTHOR(S): Ried, Walter; Grabosch, Joachim

CORPORATE SOURCE: Univ. Frankfurt a. M., Germany

SOURCE: Chemische Berichte (1956), 89, 2684-7
CODEN: CHBEAM; ISSN: 0009-2940

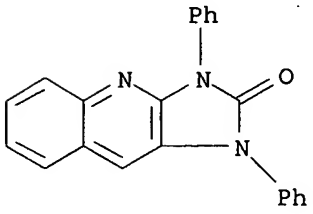
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Refluxing 0.37 g. 2-anilino-3-aminopyridine (I) in 9 cc. EtOH 15 min. with 0.17 g. Ac2 in 3 cc. absolute EtOH and adding a small amount of H2O yield 12%) 2-methyl-3-methylene-4-phenyl-3,4-dihydro-1,4,5-triazanaphthalene, fine dark red needles, m. 152°. Similarly, 0.37 g. I and 0.3 g. AcBz in 12 cc. EtOH give 5.5% 2,4-diphenyl-3-methylene-3,4-dihydro-1,4,5-triazanaphlhalene, red crystals, m. 325-7°. Refluxing 0.94 g. 2-cyclohexylamino-3-aminopyridine 1.5 hrs. in 36 cc. Ac2O yields the di-Ac derivative, prisms, m. 199-200°. Heating 6 g. 2-chloro-3-aminoquinoline (II) and 18 g. PhNH2 20 hrs. at 190-210°, steam distilling the mixture, washing the residue neutral, extracting it with Et2O, and recrystg. the Et2Oinsol. residue from m-C6H6Me6 give 65-75% 2,3-dianilinoquinoline (III), m. 214-15°, which is also obtained in 51.7% yield when 1 g. II is refluxed 15 min. with 5 cc. PhNH2 (dipicrate, m. 255°; di-Ac derivative, stout prisms, m. 28990°; di-NO derivative, pale yellow crystals, prepared with NaNO2 in AcOH). Treating 2 g. III in 30 cc. m-C6H6Me6 1.5 hrs. at 130° with COCl2, washing the precipitate with 2N NaOH, and recrystg. it from AcOH give 18.5% 1,3-diphenylquinolino[2',3',4,5]-2-imidazolone, felted yellow needles, m. 229-30°.

IT **116600-20-5**, 2H-Imidazo[4,5-b]quinolin-2-one, 1,3-dihydro-1,3-diphenyl- .

(preparation of)
RN 116600-20-5 CAPLUS
CN 2H-Imidazo[4,5-b]quinolin-2-one, 1,3-dihydro-1,3-diphenyl- (6CI) (CA INDEX NAME)

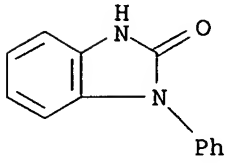


L25 ANSWER 431 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1957:12853 CAPLUS
DOCUMENT NUMBER: 51:12853
ORIGINAL REFERENCE NO.: 51:2748h-i,2749a-c
TITLE: The oxidation of diphenylurea by alkaline hypochlorite
AUTHOR(S): Rosnati, Luigi
CORPORATE SOURCE: Industria Chimica dott. Saronio, Melegnano, Italy
SOURCE: Gazzetta Chimica Italiana (1956), 86, 275-81
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

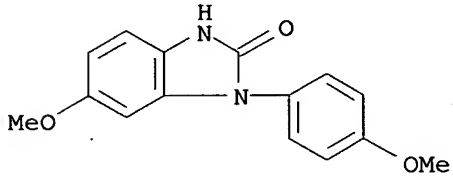
AB Although urea is definitely oxidized to N_2H_4 by NaClO, previous references to the oxidation of N,N'-derivs. of urea are uncertain or contradictory, and the present work represents the first clearly defined results. Aqueous 10% NaClO (11.1 g.), added dropwise (during 25-30 min.) to a suspension of 10.6 g. $OC(NHPh)_2$ in 300 cc. MeOH and 4 g. NaOH in 15 cc. H_2O (keeping the temperature not above 35°), the brown-yellow solution let stand 12 hrs., neutralized with HCl (litmus), evaporated to 0.5 volume, 500 cc. H_2O added, acidified with HCl (Congo red), the precipitate washed, dissolved in 400 cc. boiling 10% NaOH, C added, filtered hot, acidified with HCl, and the precipitate (8.9 g.) purified by PhMe, gives 1-phenyl-2-hydroxybenzimidazole (I), m. 201-2°, stable toward oxidizing agents, acids, and alkalies, even at elevated temps. Treatment with NaOAc-Ac_2O gives, from EtOH, 1-phenyl-2-acetoxybenzimidazole, m. 134.5-5.5°, and with BzCl-C_5H_5N gives 1-phenyl-2-benzoylbenzimidazole, m. 170°. o-$H_2NC_6H_4NHPh.HCl$ (18.5 g.) in 600 cc. H_2O and 10 g. KCNO in 50 cc. H_2O, heated 10 min. at 75°, and the precipitate purified by 30% EtOH and PhMe, give 20 g. crude o-$PhHNC_6H_4NHCONH_2.HCl$ (II). II (2.3 g.) raised during 15-20 min. to 170°, held at 170-80° until no more NH_3 is evolved (40 min.), the product dissolved in 50 cc. hot 10% KOH, the brown solution filtered with C, acidified with HCl, the precipitate washed until neutral, and the residue (1.7 g. = 81%) purified by PhMe, gives I. Following the procedure for I, 5.7 g. $(p\text{-}ClC_6H_4NH)_2CO$ gives 5.2 g. 1-(p-chlorophenyl)-2-hydroxy-6-chlorobenzimidazole, m. 236-7° (from PhMe). 1-(4-Chlorophenyl)-2-acetoxy-6-chlorobenzimidazole, m. 176-7°. $(o\text{-}MeC_6H_4NH)_2CO$ (8 g.) gives 6.8 g. 1-(o-tolyl)-2-hydroxy-4-methylbenzimidazole, m. 266-6.5° (from EtOH). $(p\text{-}MeOC_6H_4)_2CO$ (18 g.) gives 9.7 g. of 1-(4-methoxyphenyl)-2-hydroxy-6-methoxybenzimidazole, light brown, m. 245-6° (from iso-BuOH). If the H atoms on the N or those of the Ph groups in o-position to the N are replaced by Me groups, there is no reaction; e.g., neither $(PhMeN)_2CO$ nor $(2,4,6\text{-}Me_3C_6H_2NH)_2CO$ react under conditions where $OC(NHPh)_2$ is oxidized. The reaction takes place only in alc. medium; in H_2O, $OC(NHPh)_2$ remains unaltered, perhaps because of its insoly. The mechanism of the reaction is discussed.

IT **14813-85-5**, 2-Benzimidazolol, 1-phenyl-
(esters)

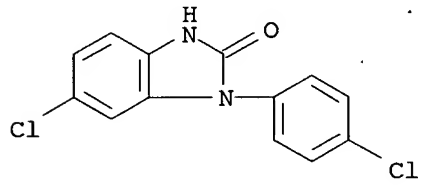
RN 14813-85-5 CAPLUS
CN 2H-Benzimidazol-2-one, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



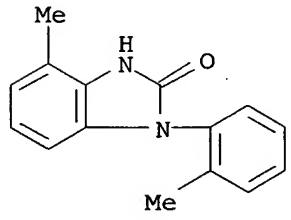
IT **19950-86-8**, 2-Benzimidazolol, 6-methoxy-1-(p-methoxyphenyl)-
19950-87-9, 2-Benzimidazolol, 6-chloro-1-(p-chlorophenyl)-
100968-99-8, 2-Benzimidazolol, 4-methyl-1-o-tolyl-
(preparation of)
RN 19950-86-8 CAPLUS
CN 2-Benzimidazolinone, 6-methoxy-1-(p-methoxyphenyl)- (8CI) (CA INDEX NAME)



RN 19950-87-9 CAPLUS
CN 2H-Benzimidazol-2-one, 6-chloro-1-(4-chlorophenyl)-1,3-dihydro- (9CI) (CA INDEX NAME)



RN 100968-99-8 CAPLUS
CN 2-Benzimidazolol, 4-methyl-1-o-tolyl- (6CI) (CA INDEX NAME)



L25 ANSWER 432 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1956:69457 CAPLUS
DOCUMENT NUMBER: 50:69457
ORIGINAL REFERENCE NO.: 50:13041a-h
TITLE: Reactions of hydrazine with heterocyclic 1,2-dicarboxylic acid esters

AUTHOR(S): Jones, Reuben G.
CORPORATE SOURCE: Lilly Research Labs., Indianapolis, IN
SOURCE: Journal of the American Chemical Society (1956), 78, 159-63
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 50:69457

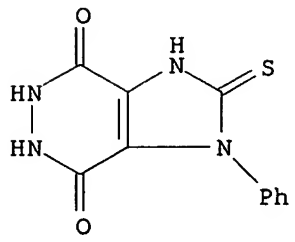
AB The appropriate dicarboxylic acid ester (0.1 mole) in 25-50 cc. MeOH treated with 15 g. $N_2H_4.H_2O$, kept several hrs. at room temperature, heated 0.5 hr. on the steam bath, and evaporated, the residue dissolved in 50-500 cc. H_2O containing 5 cc. concentrated NH4OH, the solution filtered and acidified with excess AcOH or HCl, and the crystalline precipitate washed and dried gave the following condensation products (m.p. and % yield given): 5,8-dihydroxy-1,4,6,7-tetrazanaphthalene (I), 280° (decomposition), 95; 1,3-dimethyl-5,8-dihydroxy-2,6,7-triazanapkthalene, 302° (decomposition), 97; 2-NH_2 derivative of I, above 400°, 93; 2-cyano-3-methyl-5,8-dihydroxy-4,6,7-triazanaphthalene, 320° (decomposition), 85; 2-cyano-3,8-dimethyl-5-hydroxy-4,6,7-triazanaphthalene, 338-40°, 89; 1,4-dimethyl-5,8-dihydroxy-2,3,6,7-tetrazanaphthalene, 320° (decomposition), 73; 4,7-dihydroxy-2-thia-5,6-diazaindene, 328-30°, 92; 2-methyl-4,7-dihydroxy-1-thia-5,6-diazaindene, 294-5°, 90; 1-methyl-4,7-dihydroxy-2-oxa-5,6-diazaindene (II), 282-3°, 77; 3-Me derivative of II, 345° (decomposition), 83; 1-phenyl-2-methyl-4,7-dihydroxy-1,5,6-triazaindene, 335-7°, 89; 1-phenyl-4,7-dihydroxy-1,2,5,6-tetrazaindene, 315-16°, 61; 2-mercapto-4,7-dihydroxy-1,3,5,6-tetrazaindene (III), above 400°, 67; 1-methyl-4,7-dihydroxy-1,3,5,6-tetrazaindene, 354-6°, 78°; 1-Me derivative of III, above 330°, 93; 1-phenyl-4,7-dihydroxy-1,3,5,6-tetrazaindene (IV), 315-16°, 89°; 2-SH derivative of IV, 367° (decomposition), 97. The appropriate dicarboxylic dihydrazide (0.05 mole) refluxed 2-8 hrs. with 50 cc. $N_2H_4.H_2O$ or heated 9-72 hrs. on the steam bath, the solution evaporated in vacuo on the steam bath, the solid residue dissolved in about 50-200 cc. hot H_2O, and the solution acidified with AcOH or HCl and cooled gave the following condensation products (m.p. and % yield given): 2-methyl-4,7-dihydroxy-1-oxa-5,6-diazaindene (V), 290-2°, 96; 4,7-dihydroxy-2,5,6-triazaindene (VI), above 310°, 90; 2-Me derivative (VII) of VI, 339-40°, 89; 1,5,6-isomer of V, 355° (decomposition), -; 4,7-dihydroxy-1,3,5,6-tetrazaindene (VIII), above 400°, 92. The appropriate dihydrazide (0.05 mole) in 100 cc. 2N HCl heated 6 hrs. on the steam bath, cooled, and filtered gave the following condensation products: 4,7-dihydroxy-2-oxa-5,6-diazaindene, above 300°, 70; V; VI; VII; VIII. The appropriate diester (0.1 mole) in about 50 cc. MeOH allowed to stand several hrs. with 15 g. $N_2H_4.H_2O$ or heated 0.5 hr. on the steam bath, and cooled, and the product recrystd. from H_2O or EtOH or dissolved in dilute acid and repptd. with NH4OH gave the corresponding dicarboxylic acid dihydrazides (IX) of the following acids (m.p. and % yield of the IX given): 4,5-imidazoledicarboxylic acid, above 375°, 99; 3,4-pyrazoledicarboxylic acid, above 300°, 98; 3,4-furandicarboxylic acid (X), 270° (decomposition), 88; 5-methyl-2,3-furandicarboxylic acid, m. 190°, 94; 3,4-pyrroledicarboxylic acid (XI), above 300°, 95; 1-Me derivative of XI, 330° (decomposition), 90. Dihydrazide of X (16 g.) and 25 cc. $N_2H_4.H_2O$ heated 6 hrs. on the steam bath, the brown solution evaporated in vacuo, the residue dissolved in 100 cc. dilute aqueous NaOH, and the solution treated with C and acidified with AcOH gave 13 g. 3,3'-dihydroxy-4,4'-bipyrazole (XII), darkened at 360° but did not melt (from H_2O); XII was also obtained in 50% yield from di-Et 1-formyl-2-diethoxymethylsuccinate in EtOH with excess N_2H_4. 1-Methyl-4,7-dihydroxy-2-oxa-5,6-diazaindene (XIII) (10 g.) heated 8 hrs.

on the steam bath with 20 cc. N2H4.H2O gave 90% 5-Me derivative of XII, m. above 360° (sublimed at 275° and 0.1 mm.). The 3-Me derivative of XIII gave similarly the 5,5'-di-Me derivative of XII, m. above 375°, in 52% yield when refluxed 15 hrs. with N2H4.

IT **63886-80-6**, 1H-Imidazo[4,5-d]pyridazine-4,7-diol, 2-mercapto-1-phenyl-
(preparation of)

RN 63886-80-6 CAPLUS

CN 1H-Imidazo[4,5-d]pyridazine-4,7-dione, 2,3,5,6-tetrahydro-1-phenyl-2-thioxo- (9CI) (CA INDEX NAME)



L25 ANSWER 433 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1956:69372 CAPLUS

DOCUMENT NUMBER: 50:69372

ORIGINAL REFERENCE NO.: 50:12987i,12988a-i,12989a-i

TITLE: Anhydro compounds from nitrogen-containing derivatives of thioglycolic acid. II. Imidazole and benzimidazole compounds

AUTHOR(S): Duffin, G. F.; Kendall, J. D.

CORPORATE SOURCE: Ilford Ltd., Ilford, UK

SOURCE: Journal of the Chemical Society, Abstracts (1956) 361-8
CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 45, 9057g. (2-Benzimidazolylthio)acetic acid (I) with Ac2O gave benzimidazolo[2',1',2,3]thiazolidin-4-one (II) from which merocyanine dyes were prepared The 1-substituted derivs. of I, like the corresponding quinoline compds., gave stable anhydro compds. which usually gave products derived by attack of the reagent at 2 different points in the molecule. No anhydro compds. corresponding to those derived from (2-quinolylthio)propionic and -butyric acid could be obtained from the α-Me (III) or α-Et (IV) derivs. of I. I (10 g.), 15 cc. C5H5N, and 10 cc. Ac2O heated 10 min. on a steam-bath gave 5.8 g. II, m. 181° (from EtOH), λ 238, 282, 291 mμ (ε 18,900, 10,300, and 8900) (all absorption maximum were determined in alc.). II (9.5 g.), 12 cc. HC(OEt)3, and 15 cc. Ac2O refluxed 20 min. and evaporated in vacuo yielded 5.6 g. 5-ethoxymethylenebenzimidazolo[2',1',2,3]thiazolidin-4-one (V), plates, m. 167-9°. II (0.475 g.), 0.81 g. 2-methylthiobenzothiazole-MeI, 25 cc. EtOH, and 0.5 cc. NEt3 refluxed 10 min. gave 0.68 g. 5-(2,3-dihydro-3-methyl-2-benzothiazolylidene)benzimidazolo[2',1',2,3]thiazolidin-4-one, m. 330° (from dioxane). The following were similarly obtained: II and 2-(2-acetanilidovinyl)benzothiazole-EtI gave 64% 5-[2-(3-ethyl-2,3-dihydro-2-benzothiazolylidene)ethylidene]benzimidazolo[2',1',2,3]thiazolidin-4-one (VI), red needles, m. 290° (from dioxane). VI was obtained in 56% yield from V and 2-methylbenzothiazole-EtI. The 5-[2-(2,3-dihydro-3-methyl-2-bensoxazolylidene)ethylidene] analog [from II and 2-(2-ethylthiovinyl)benzoxazole metho-p-toluenesulfonate] as orange

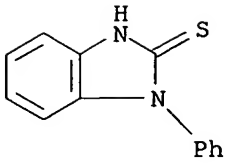
needles, m. 318° (from dioxane), in 60% yield. The 5-[2-(1,3,3-trimethyl-2 indolinylidene)ethylidene]analog [from II and 2-(2-acetanilidovinyl)-3,3-dimethylindolenine-MeI] 42% yield as orange needles, m. 252° (from MeOH). The 5-[2-(1,4-dihydro-1-methyl-4-quinolinylidene)ethylidene] analog [from II and 4-(2-ethylthiovinyl)quinoline-MeI], dark blue plates, m. 295° (from MeOH), was prepared in 57% yield. The 5-[2-(1,2-dihydro-1-methyl-2-quinolinylidene)-ethylidene] analog [from II and 2-(2-ethylthiovinyl)quinoline-MeI] in 67% yield as red needles, m. 339° (from alc.). The 5-benzylidene, yellow plates, in 25% yield, m. 219° (from C6H6), and the 5-p-dimethylaminobenzylidene analog in 45% yield, orange needles, m. 269° (from alc.).
2-Aminodiphenylamine (VII) (9.2 g.) and 3.25 g. NaCNO refluxed 2 hrs. in EtOH-10N HCl yielded 6.1 g. 2-ureidodiphenylamine (VIII), plates, m. 157°. VIII (5 g.) heated 1 hr. at 160° evolved NH3 and gave 2.8 g. 2-hydroxy-1-phenylbenzimidazole (IX), m. 204°. By a similar process N-methyl-o-ureidoaniline(?) (X) was prepared in 52% yield from N-methyl-o-phenylenediamine (XI) as plates, m. 180°. X on heating gave 70% 2-hydroxy-1-methylbenzimidazole (XII), plates, m. 188°. XII was identical with the product from XI and COCl2.
N-Methyl-o-nitroaniline (56.8 g.) in EtOH and 20% NaOH treated 20 min. with 100 g. Zn dust, the mixture refluxed until colorless, filtered hot, the solid washed with EtOH, and the filtrate refluxed 4 hrs. with 48 cc. CS2 gave 50 g. 1-methylbenzimidazole-2-thiol (XIII), m. 195°. Benzimidazole-2-thiol (XIV) (87%) and 1-phenylbenzimidazole-2-thiol (XV) (70%), m. 194° were similarly obtained from CS2 with o-C6H4(NH2)2 and VII, resp. XIII (8.2 g.) in 50 cc. N NaOH shaken 1 hr. with 3.2 cc. MeI, extracted with CHCl3, concentrated, and distilled gave 6.5 g. 1-methyl-2-(methylthio)benzimidazole (XVI), plates, m. 56°, b0.8 112-15°, λ 253, 285, and 292 mμ (ε 6500, 13,600, and 14,200). XVI heated 2 hrs. with MeI gave 1,3-dimethyl-2-methylthiobenzimidazolium iodide (XVII), m. 152°. XVII (1.5 g.) refluxed 2 hrs. with 5 cc. C5H5N yielded 0.5 g. 2,3-dihydro-1,3-dimethyl-2-thiobenzimidazole, m. 153-4°, λ 254, 309 mμ (ε 18,100 and 29,500). 2-Methylamino-5-nitroaniline (28 g.), 9.8 g. KOH, 80% EtOH, and 28 cc. CS2 refluxed 20 hrs., diluted with H2O, the EtOH removed, and the hot residue added to 280 cc. N HCl yielded 30.2 g. 1-methyl-5-nitrobenzimidazole-2-thiol, m. 304-5° (decomposition). 5-Nitro-1-phenylbenzimidazole-2-thiol similarly obtained in 69% yield, yellow needles, m. 282°. 1-Methylimidazole-2-thiol (5.7 g.), 4.8 g. ClCH2CO2H, and H2O refluxed 1 hr., 50 ml. N NaOH added, the solution concentrated to dryness, and the residue extracted gave 7.1 g. (1-methyl-2-imidazolylthio)acetic acid (XVIII), m. 85°, λ 255 mμ (ε 20,600). The following exemplifies the procedure for preparing derivs. of I, 5-XC6H3.NR.C(SCHR'CO2H):N(XVIIIa). XIII (16.4 g.), 80 cc. 10% NaOH, 9.5 g. ClCH2CO2H heated 2 hrs. on the steam bath, the hot solution filtered, acidified with concentrated HCl, and the precipitated 1-Me derivative (XIX) of I recrystd. from EtOH in 75% yield, m. 190°, λ 283, 291 mμ (ε 13,400 and 13,900). Analogous XVIIIa were (R, R', X, compound number, m.p., and % yield given): H, H, H, I, 211°, 67; Ph, H, H, XX, 176°, 60; Ph, Me, H, -, 97°, 39; Ph, Et, H, XXI, 87°, 32; Ph, H, NO2, XXII, 234-5°, 67; Me, H, NO2, XXIII, 235°, 30. XIII (9.2 g.) and 9.3 g. EtCHBrCO2H refluxed 6 hrs. in H2O, cooled, and 40% NaOH added gave 7.9 g. α-(1-methyl-2-benzimidazolylthio)butyric acid (XXIV), m. 132° (from aqueous alc.). α-(1-Methyl-2-benzimidazolylthio)propionic acid (XXV) was obtained in a similar process as needles, m. 131° (from H2O) in 61% yield. XVIII (6 g.), 18 ml. C5H5N, and 6 ml. Ac2O warmed 5 min. gave 4.25 g. anhydro compound, m. 201°, λ 238, 334 mμ (ε 3400 and 9900), λC6H6 335 mμ (ε 10,900), λaq.C5H5N 337 mμ (ε 36,700). In 15 min. XIX (5 g.) similarly yielded 3.6 g. anhydro compound (XXVI), m. 255°, insol. in all the usual solvents.

XX similarly gave 44% anhydro compound (XXVII), m. 222° (from xylene) (64% yield by refluxing XX with twice its weight of Ac2O), λ 255, 286, 293, and 350 mμ (ε 12,000, 7900, 7800, and 9700), λdioxane 270, 287, 294, and 360 mμ (ε 11,500, 7500, 7500, and 7500), λC6H6 288, 295, and 365.5 mμ (ε 8100, 8200, and 6950), λaq.C5H5N 292 and 352 mμ (ε 6850 and 10,500). By similar reactions XXIII gave an anhydro compound (XXIX) as orange needles, m. 238° (decomposition) (81% yield), and XXII gave 62% anhydro compound (XXX), yellow needles, m. 221°. XXVII (5 g.) heated at 100° with 20 cc. 50% H2SO4, solution occurred with evolution of CO2, extracted with C6H6, the C6H6 treated with 2N Na2CO3, and the carbonate solution on acidification gave 0.87 g. XX; further extraction with N NaOH gave 0.03 g. XX. Removal of the C6H6 gave 2.6 g. of sticky solid which on purification afforded 2.1 g. 1-phenyl-2-benzimidazolyl α-(1-phenyl-2-benzimidazolylthio)thiolacetate (XXXI), plates, m. 176° (from C6H6EtOH), λ 250, 285, and 292 mμ (ε 24,800, 21,800, and 21,500). XXXI (2 g.) refluxed 1 hr. with 10% EtOH-NaOH yielded 0.7 g. XV and 1 g. XX. Under similar conditions XXIX and XXX gave XXIII and XXII only, in yields of 87% and 92%, resp. XXVII (2.5 g.), 80 cc. H2O, and 10 cc. HNO3 (d. 1.41) refluxed 1 hr. gave 1.2 g. 2-hydroxy-5-nitro-1-phenylbenzimidazole (XXXII), m. 239-40° (from aqueous alc.). XXXII was identical with the compound derived (45%) from XXX. Basification of the original acid filtrate gave an oil from which was derived the picrate of 1-phenylbenzimidazole (XXXIII), identical with that prepared from authentic XXXIII. By a similar process XXVI gave 28% 1-methylbenzimidazole picrate, m. 244°, and 31% 2-hydroxy-1-methyl-5-nitrobenzimidazole (XXXIV), m. 302° (from AcOH). XXXIV was identical with the compound obtained in 40% from XXIX and dilute HNO3. By similar reactions with dilute HNO3 XV gave 80% XXXIII as the picrate, IX gave 63% XXXII, and XX gave 83% recovered material. XXVII (2.5 g.) refluxed 1 hr. with 40% NaOH and EtOH gave 1.8 g. of material, m. 161° which was identical with the equimolar eutectic from IX and XV by dissn. in alkali and repptn. with acid or by recrystn. from aqueous alc. or C6H6-light petroleum. By a similar process XXVI gave 68% XIII. XXVII (5 g.), EtOH, and concentrated HCl treated with 5 g. Zn amalgam liberated H2S, MeSH, and CO2 gave 3.1 g. XV. XXVII (5.5 g.) and 10 g. PhCH2NH2 refluxed 1 hr. gave 2.2 g. benzimidazole-2-thiol, evaporation of the Et2O gave 1.49 g. 2-benzylamino-1-phenylbenzimidazole (XXXV), m. 145°. PhCH2NH2 and the parent compound likewise gave 77% XXXV, but XV was recovered in 88% after 2 hrs. refluxing with excess PhCH2NH2. The 1-Ph derivative of IV (2 g.) and Ac2O refluxed 1 hr. gave 0.7 g. 3-acetyl-2,3-dihydro-1-phenyl-2-thioxobenzimidazole (XXXVI), m. 191° (from Me2CO), λ 312 mμ (ε 20,800). XXXVI was obtained in 78 and 50% yields from Ac2O and XV or the 1-Ph derivative of III, resp. 3-Acetyl-2,3-dihydro-1-methyl-2-thioxobenzimidazole was obtained (72%, 15%, and 28%) similarly from Ac2O and XIII, XXV, or XXIV. It recrystd. from Me2CO as needles, m. 144°, λ 241 and 310 mμ (ε 17,100 and 21,500).
The 1-Ph derivative of IV (5 g.) in 6 cc. C5H5N and 5 cc. Ac2O gave 3.07 g. 1-phenyl-2-benzimidazolyl α-(1-phenyl-2-benzimidazolylthio)thiolbutyrate (XXXVII), plates, m. 147° (from C6H6-light petroleum), λ 242, 285, and 292 mμ (ε 22,000, 19,400, and 18,600). XXXVII refluxed with 10% alc. NaOH gave 85% 1-Ph derivative of IV and 85% XV. Refluxing Ac2O converted XXXVII into 68% XXXVI.

IT **4493-32-7**, 2-Benzimidazolethiol, 1-phenyl-
(and esters)

RN 4493-32-7 CAPLUS

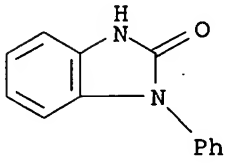
CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



IT **14813-85-5**, 2-Benzimidazolol, 1-phenyl- **31918-27-1**, 2-Benzimidazolol, 5-nitro-1-phenyl- **634167-34-3**, 2-Benzimidazolinethione, 1-acetyl-3-phenyl- **733031-20-4**, 2-Benzimidazolethiol, 5-nitro-1-phenyl-
(preparation of)

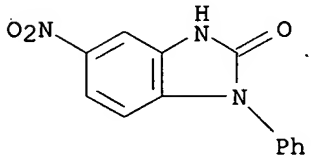
RN 14813-85-5 CAPLUS

CN 2H-Benzimidazol-2-one, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



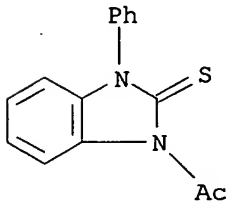
RN 31918-27-1 CAPLUS

CN 2H-Benzimidazol-2-one, 1,3-dihydro-5-nitro-1-phenyl- (9CI) (CA INDEX NAME)



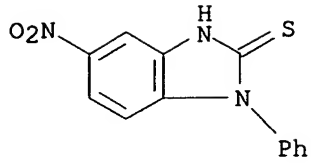
RN 634167-34-3 CAPLUS

CN 2H-Benzimidazole-2-thione, 1-acetyl-1,3-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



RN 733031-20-4 CAPLUS

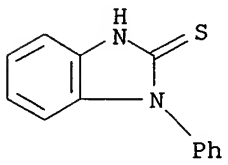
CN 2H-Benzimidazole-2-thione, 1,3-dihydro-5-nitro-1-phenyl- (9CI) (CA INDEX NAME)



L25 ANSWER 434 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1956:62679 CAPLUS
DOCUMENT NUMBER: 50:62679
ORIGINAL REFERENCE NO.: 50:11714h-i
TITLE: Stabilized polyethylene compositions
INVENTOR(S): Vincent, John R.; Vincent, Margaret B.
PATENT ASSIGNEE(S): E. I. du Pont de Nemours & Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2727879		19551220	US	

AB The addition of 0.2-5% of a 2-mercaptoaryleneimidazole, e.g. 2-mercaptobenzimidazole (I), as a stabilizer to polyethylene increases its resistance to weathering in strong sunlight. Thus, an C2H4 polymer containing only 0.05% I as a stabilizer required 6 months of exposure in Florida sunlight for its elongation to be decreased from 600 to 200%. Increasing the amount of I to 0.5-1.0% stabilized the polymer for 18 months of exposure. The action of I was not generally adversely effected by other materials which may be added to the polymer. Comparative data show superiority of these compds. to other inhibitors.
IT **4493-32-7**, 2-Benzimidazolethiol, 1-phenyl-
(as ethylene-polymer light stabilizer)
RN 4493-32-7 CAPLUS
CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



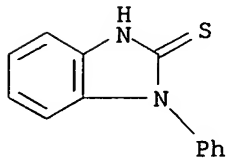
L25 ANSWER 435 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1949:40965 CAPLUS
DOCUMENT NUMBER: 43:40965
ORIGINAL REFERENCE NO.: 43:7362b-c
TITLE: Studies on addition agents for photographic emulsions and developers. II. Properties of derivatives of mercaptobenzimidazole as addition agents
AUTHOR(S): Oyama, Yasushi
SOURCE: Rikagaku Kenkyusho Iho (1943), 22, 483-9
CODEN: BPYCA6; ISSN: 0366-2608
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Several derivs. of 2-mercaptobenzimidazole (I) were prepared and added to photographic emulsions and to developers. I and its N-Ph derivs.

interfere with development and give a warm tone on chloride emulsions. S-alkyl substitution causes disappearance of such interfering effects and at the same time allows development of chloride emulsions in fairly good blue-black tones. The fog-inhibiting properties of S-alkyl derivs. were fairly strong.

IT **4493-32-7**, 2-Benzimidazolethiol, 1-phenyl-
(in photographic emulsions and developers)

RN 4493-32-7 CAPLUS

CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



L25 ANSWER 436 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1949:40964 CAPLUS

DOCUMENT NUMBER: 43:40964

ORIGINAL REFERENCE NO.: 43:7361c-e,7362a-b

TITLE: Studies on addition agents for photographic emulsions and developers. I. The relation between chemical constitution and photographic properties of organic addition agents

AUTHOR(S): Oyama, Yasushi

SOURCE: Rikagaku Kenkyusho Iho (1942), 21, 364-74
CODEN: BPYCA6; ISSN: 0366-2608

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

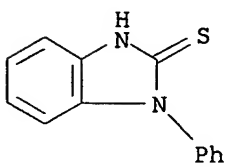
GI For diagram(s), see printed CA Issue.

AB Organic addition agents for photographic emulsions and developers were classified according to the relation between chemical constitution and photographic properties. O. concludes that: (1) All of these agents, with some exceptions, have the property of making salts or double salts with Ag ions or Ag salts, and even the exceptions react in close connection with compds. that have this property. (2) They generally have linkages including N, S, O, or halogen atoms, and the most effective is the group N Y C-X, where X and Y are N, S, O, C:C, etc. (3) Chemical constitution governs the production of certain useful Ag salts, and their usefulness is governed by their phys. and chemical properties. (4) For sensitizers the group -NC:S and for addition agents for blue-black developing the groups :NNHC(:S)N: or :NN:C(NH2)N: in chain compds. and -N:NN: or -XC:N- for ring compds. are necessary but are insufficient in themselves. (5) An addition agent usually exhibits 2 or more of these effects, which are generally independent of each other.

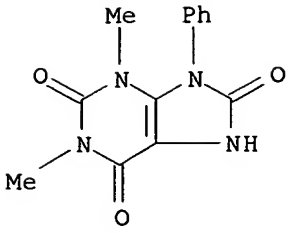
IT **4493-32-7**, 2-Benzimidazolethiol, 1-phenyl-
(in photographic emulsions and developers)

RN 4493-32-7 CAPLUS

CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



L25 ANSWER 437 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1924:13537 CAPLUS
DOCUMENT NUMBER: 18:13537
ORIGINAL REFERENCE NO.: 18:1816e-i,1817a
TITLE: Action of alkali on substituted uric acids I. 1,3-Dimethyl-9-phenyluric acid
AUTHOR(S): Gatewood, Elizabeth Stuart
SOURCE: Journal of the American Chemical Society (1923), 45, 3056-64
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 18:13537
GI For diagram(s), see printed CA Issue.
AB 1,3-Dimethyl-9-phenyluric acid (I) is decomposed only very slowly by 4 N alkali at room temperature; at 100° with more dilute alkali, the decomposition is more rapid and with 4 N alkali it is instantaneous; the products are MeNH2, CO2 and 3- phenylisohydantoin-5-carboxylic methylamide, NH.CO.NPh.C(OH):CCONHMe (II). When warmed with alkali, or even on standing about an hr. with cold alkali, II decomps. completely into PhNHCONH2, MeNH2, (CO2H)2 and HCO2H; the PhNHCONH2 seps. after only 15 min. but no (CO2H)2 can yet be detected at this point unless the solution is first warmed, indicating that its formation is due to a secondary reaction; probably OHCCO2H is first formed and changes into (CO2H)2 and HOCH2CO2H when heated or allowed to stand with the alkali. With H2O2 in dilute alkaline solution II yields 3-phenyl-5-hydroxyhydantoin-5-carboxylic methylamide, NH.CO.NPh.CO.C(OH)CONHMe (III), which is instantly decomposed by cold alkali into PhNHCONH2 and HO2CCOCONHMe (IV) and on boiling is further decomposed into MeNH2, PhNHCONH2 and CO(CO2H)2 (V). II (1.2-1.4 g. from 2 g. I in 100 cc. of 4 N NaOH slowly heated to boiling, boiled 0.5 min., cooled slightly, acidified with HCl and allowed to stand), rectangular plates, α 1.571, γ 1.629, m. 249-50°, gives with boiling Ac2O a substance m. 185-7°, does not react with PhNCO at 165° or in alkaline solution at 0°. III (0.6 g. from 1 g. II in 12 cc. H2O with 2.9 g. KOH and 70 cc. of 3% H2O2 kept 5 min. below 10° and then acidified with HCl), rectangular plates, α 1.545, γ 1.583, m. 194-5°; the mother liquors yield a substance separating in needles, α 1.556, γ 1.695, m. 188-90°. The phenylhydrazone of V seps. in needles, α 1.459, γ 1.800, m. 165°; that of IV in hexagonal plates, α 1.600, γ 1.715, m. 167° (Torrey, Ber. 31, 2162 (1898), gives 158°). Et phenyloxalurate (4.7 g. from 5 g. NH2COCO2Et and 10 g. PhNCO heated 1 hr. at 110-2°), m. 125-6° (gas evolution), seps. in 2 crystalline forms, α 1.590, γ 1.680, and α 1.675, γ 1.755, resp.; 1 g. allowed to stand in H2O 0.5 hr. with 1 g. of 33% MeNH2 gives 0.74 g. of the methylamide, m. 210-5°, α 1.595, γ 1.700, instantly decompd, by cold 4 N NaOH into PhNHCONH2, (CO2H)2 and MeNH2. 1,7-Di-methyl-9-phenylpseudouric acid (8 g. from 5 g. 1.7-dimethyluramil in 60 cc. of N KOH treated at 0-2° in the course of 0.5 hr. with 3.8 g. PhNCO), turns pink 160°, light yellow 210°, m. 220°, dissolves in about 350 parts H2O, seps. in hexagonal plates, α 1.555, γ 1.695; 5 g. boiled in 1 l. of 20% HCl until crystallization begins and concentrated yields 3.8 g. 1,7-dimethyl-9-phenyluric acid, rectangular and hexagonal plates, α 1.540, γ 1.755, does not m. 280°, is unchanged by boiling 10 min. with 4 N alkali, is also obtained in 0.5 g. yield, together with 0.1 g. of the 1,3,7-Me3 acid, from 1 g. of 7-methyl-9-phenyluric acid with 2 g. Me2SO4 in 2 N NaOH.
IT **22305-92-6**, Uric acid, 1,3-dimethyl-9-phenyl-
(reaction with NaOH)
RN 22305-92-6 CAPLUS
CN Uric acid, 1,3-dimethyl-9-phenyl- (8CI) (CA INDEX NAME)



L25 ANSWER 438 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1923:2983 CAPLUS
DOCUMENT NUMBER: 17:2983
ORIGINAL REFERENCE NO.: 17:538a-i,539a-b
TITLE: Purines. IV. Action of hydrogen peroxide upon certain phenyl-substituted uric acids
AUTHOR(S): Moore, F. J.; Gatewood, Elizabeth S.
SOURCE: Journal of the American Chemical Society (1923), 45, 135-45
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

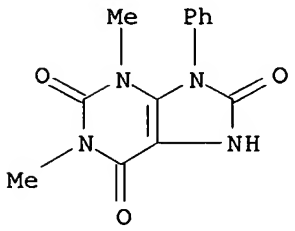
AB cf. C. A. 12, 1782. It was shown in the earlier papers that H2O acting upon uric acid (A) in a solution whose alkalinity is less than 1 N and temperature higher than 80° gives allantoin and carbonyldiurea, the latter in a solution more strongly alkaline than 0.5 N being converted into cyanuric acid (B); on the other hand, at room temperature and in solution more strongly alkaline than 1 N. the product is allantoxanic acid, which, if the solution is acidified before removing the H2O2, is oxidized to B. No intermediate product between the A and the above products was found, however, and no light was thrown upon any relationship which may exist between the mechanism of this reaction and the KMnO4 oxidation. Accordingly, the action of H2O2 upon numerous purine derivs. (theobromine, caffeine, xanthine, guanine, 3-, 7- and 9-methyl- and 7-oxymethyleneuric acids, and 3,7-dimethyl-4,5-uric acid glycol) was studied but all the results were negative in the sense that they did not invite further study; some of the compds. were unaffected, some were decomposed by the alkali; still others gave jelly-like mixts. 9-Phenyluric acid (C), however, finally gave homogeneous products in reasonable yields, viz., NH3, (CO2H)2, PhNHCONH2, asym-phenylbiuret (D) and a compound (E) which is converted into D by NH3 and proved to be a new phenylbiuret entirely distinct from the 2 already known (see below). On the other hand, I,3-dimethyl-9-phenyluric acid (F) and 7-methyl-9-phenyluric acid (G) yield no substituted biurets but NH3, (CO2H)2 and PhNHCONHMe (H). Assuming that E is the true sym-phenylbiuret, PhN(CONH2)2, and since D is probably formed only by the transformation of E, the oxidations of C, G and F can be interpreted from a single point of view; the 1st step is regarded as consisting in the breaking of the bonds between positions 2 and 3, 4 and 5, and 5 and 7, giving E in the 1st case and in the other two the same H2NCONPhCONHMe which decomps. into NH3, CO2 and H, while the E partly undergoes a similar decomposition into PhNHCONH2 and another part is rearranged by the NH3 into D. Not too much is claimed for this interpretation; its weakest point is the fact that E on similar treatment gives no PhNHCONH2, which may, therefore, come from some other source. This, however, does not necessarily invalidate the other assumptions. This question cannot be definitely settled until the aryl substituted biurets have been thoroughly studied. 7-Methyl-9-phenylpseudouric acid (7 g. from 5 g. of 7-methyluramil in 60 cc. of N KOH at 0° treated with 5 g. PhNCS in small portions), needles, m.

245-50° to a yellow liquid, shows parallel extinction, α 1.636, γ 1.714+; 3 g. boiled with 600 cc. of 35% HCl and concentrated gives 76% of G, needles, does not m. 265°, gives the murexide reaction, extinction parallel, α 1.557, γ, 1.674+. I,3-Dimethyl-9-phenylpsezidouric acid, obtained in 28-37 g. yield from 30 g. 1,3-dimethyluramil in 360 cc. of N KOH treated below 4° in the course of 1 hr. with 30 g. PhNCS, or in 5 g. yield from 5 g. of 9-phenylpseudouric acid in 40 cc. of 2 N KOH shaken 1 hr. at 0° with 11 g. Me2SO4, plates from H2O, m. 189-90° to a red liquid, extinction 25-7°, α 1.525, γ, 1.647; on slow crystallization there seps. together with the above form a monohydrate, needles with parallel extinction, α 1.583, γ, 1.768+, 1.800-, seps. from alc. in the anhydrous form, has the same m. p. as the latter. F does not m. 300°, is readily decomposed by alkalies but is stable towards Na2CO3, seps. in rectangular or hexagonal plates with sym. extinction, α 1.155+, γ 1.684; yield, 1.3-1.6 g. from 5 g. of the pseudo acid. 9-Allylpseudouric acid (3.5 g. from 5 g. uramil in 100 cc. of N KOH at 0° treated in the course of 1 hr. with 3 g. C3H5NCS), needles, turns pink 170°, m. 227-8° (decomposition), shows parallel extinction, α 1.591, γ 1.69; 3 g. with HCl gives 2 g. 9-allyluric acid, does not m. 300°, seps. in plates with sym. extinction, α 1.75, γ 1.775, 1.80. Below are, resp., the habit, extinction and indexes (α and γ) for various cornpds. determined during the course of this work: Urea, prisms, parallel, 1.4743, 1.6005; PhNHCONH2, plates, parallel, 1.602, 1.627; CO(NHPh)2, needles, parallel, 1.583, 1.74(?); NH(CONHPh)2, needles, parallel, 1.591, < 1.656 and > 1.649; allantoin, hexagonal plates, parallel, 1.579, 1.66-; uroxanic acid, tetrahedrons, -, 1.5316, 1.6005; acid K uroxanate, long needles, parallel, 1.4676, 1.629+; spiro-dihydantoin, hexagonal plates, 25-6°, 1.571-, 1.602; NH4 chloroplatinate, thick hexagonal plates, isotropic, 1.8, -; methylammonium chloroplatinate, thin hexagonal plates, isotropic, 1.74, -.

IT **22305-92-6**, Uric acid, 1,3-dimethyl-9-phenyl- (preparation of)

RN 22305-92-6 CAPLUS

CN Uric acid, 1,3-dimethyl-9-phenyl- (8CI) (CA INDEX NAME)



=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	195.81	911.93

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-28.47	-28.47

FILE 'REGISTRY' ENTERED AT 09:35:36 ON 04 APR 2005

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 1 APR 2005 HIGHEST RN 847818-85-3
DICTIONARY FILE UPDATES: 1 APR 2005 HIGHEST RN 847818-85-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

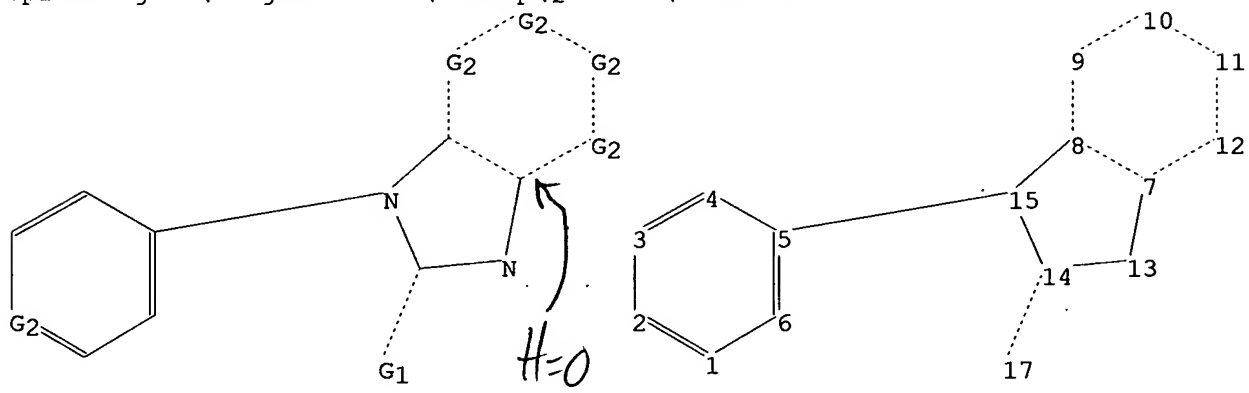
****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

Revise search-

=>
Uploading C:\Program Files\Stnexp\Queries\10681924e.str



chain nodes :
17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
5-15 14-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14
14-15
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-15 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12
13-14 14-15 14-17

G1:O,S

G2:C,N

Hydrogen count :
7:= exact 0
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS

L26 STRUCTURE UPLOADED

=> s L26
SAMPLE SEARCH INITIATED 09:36:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1703 TO ITERATE

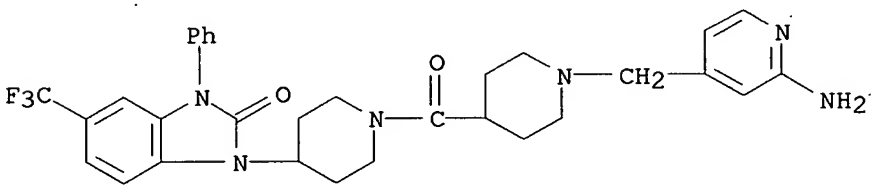
58.7% PROCESSED 1000 ITERATIONS 34 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 31585 TO 36535
PROJECTED ANSWERS: 702 TO 1614

L27 34 SEA SSS SAM L26

=> d

L27 ANSWER 1 OF 34 REGISTRY COPYRIGHT 2005 ACS on STN
RN 633311-73-6 REGISTRY
ED Entered STN: 02 Jan 2004
CN Piperidine, 1-[[1-[(2-amino-4-pyridinyl)methyl]-4-piperidinyl]carbonyl]-4-[2,3-dihydro-2-oxo-3-phenyl-5-(trifluoromethyl)-1H-benzimidazol-1-yl]-(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C31 H33 F3 N6 O2
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> s L26 full
FULL SEARCH INITIATED 09:36:33 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 34288 TO ITERATE

100.0% PROCESSED 34288 ITERATIONS 1438 ANSWERS
SEARCH TIME: 00.00.01

L28 1438 SEA SSS FUL L26

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	163.60	1075.53

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-28.47

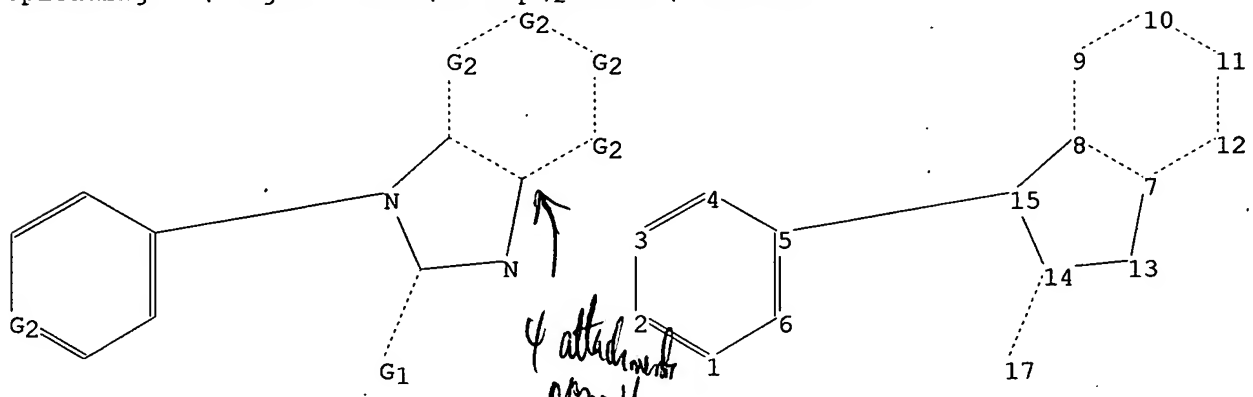
FILE 'CAPLUS' ENTERED AT 09:36:47 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 4 Apr 2005 VOL 142 ISS 15
FILE LAST UPDATED: 3 Apr 2005 (20050403/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

Revise search.

=> s L28
L29 421 L28
=>
Uploading C:\Program Files\Stnexp\Queries\10681924f.str



4 attachment non-H
H=0

chain nodes :
17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
5-15 14-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14 14-15

```
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-15  7-8  7-12  7-13  8-9  8-15  9-10  10-11  11-12
13-14  14-15  14-17


G1:O,S

G2:C,N

Hydrogen count :
7:= exact 0
Connectivity :
7:4 E exact RC ring/chain
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  17:CLASS



L30     STRUCTURE UPLOADED

=> s L30
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



SAMPLE SEARCH INITIATED 09:38:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1703 TO ITERATE

 58.7% PROCESSED    1000 ITERATIONS                                1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        31585 TO    36535
PROJECTED ANSWERS:               1 TO      112

L31           1 SEA SSS SAM L30



L32          1 L31

=> fil reg
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                   0.45    1077.31

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)        SINCE FILE      TOTAL
                                                     ENTRY    SESSION
CA SUBSCRIBER PRICE                                   0.00     -28.47

FILE 'REGISTRY' ENTERED AT 09:38:21 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 American Chemical Society (ACS)
```

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 1 APR 2005 HIGHEST RN 847818-85-3
DICTIONARY FILE UPDATES: 1 APR 2005 HIGHEST RN 847818-85-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

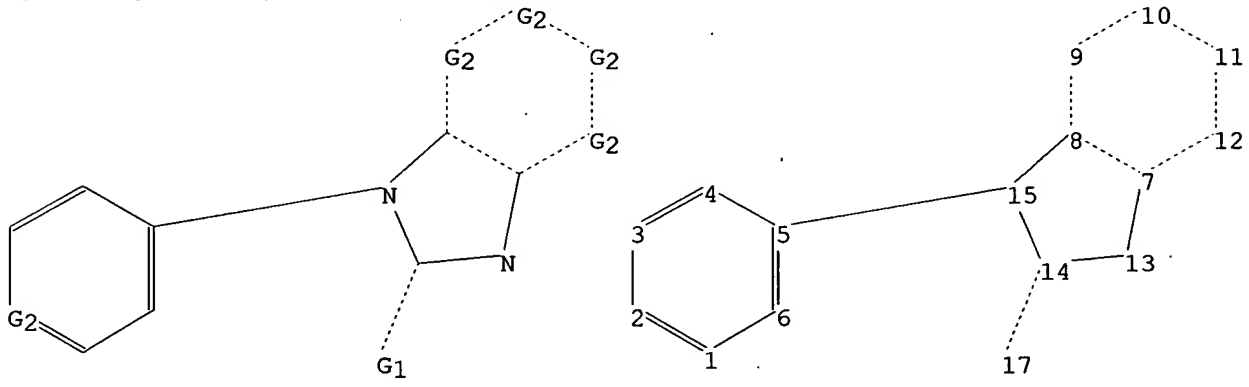
****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

Revise search

=>
Uploading C:\Program Files\Stnexp\Queries\10681924f.str



chain nodes :
17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
5-15 14-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14
14-15
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-15 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12
13-14 14-15 14-17

G1:O,S

G2:C,N

```
Hydrogen count :
7:= exact 0
Connectivity :
7:4 E exact RC ring/chain
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  17:CLASS



L33     STRUCTURE UPLOADED

=> d
L33 HAS NO ANSWERS
L33             STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s L33 full
FULL SEARCH INITIATED 09:38:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  34288 TO ITERATE

100.0% PROCESSED   34288 ITERATIONS                              39 ANSWERS
SEARCH TIME: 00.00.01

L34          39 SEA SSS FUL L33

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               161.33    1238.64

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                   ENTRY    SESSION
CA SUBSCRIBER PRICE                                0.00     -28.47

FILE 'CAPLUS' ENTERED AT 09:38:51 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 4 Apr 2005  VOL 142 ISS 15
FILE LAST UPDATED: 3 Apr 2005  (20050403/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.
```

=> s L34
L35 7 L34

=> d ibib abs hitstr 1-7

L35 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:331928 CAPLUS
DOCUMENT NUMBER: 140:357354
TITLE: A preparation of benzimidazolone derivatives useful as anti-inflammatory agents
INVENTOR(S): Dhar, T. G. Murali; Potin, Dominique; Maillet, Magali Jeannine Blandine; Launay, Michele; Nicolai, Eric Antoine; Iwanovicz, Edwin J.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004032861	A2	20040422	WO 2003-US31960	20031009
WO 2004032861	A3	20040805		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004116467	A1	20040617	US 2003-681924	20031009
PRIORITY APPLN. INFO.:			US 2002-417935P P	20021011
OTHER SOURCE(S):	MARPAT 140:357354			

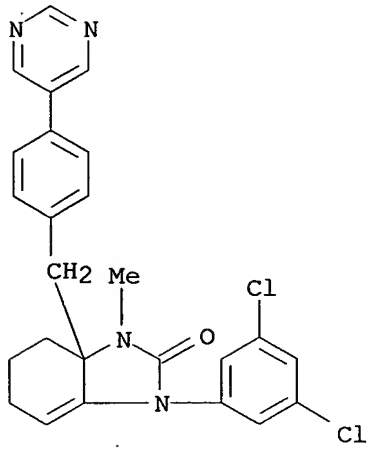
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to benzimidazolone derivs. of formula I [wherein: K is O or S; Q is a bond or C(O), etc.; Ar is (un)substituted (hetero)aryl; J1 is a bond, -N(R4)-, etc.; J2 and J3 are -N(R4)- or (un)substituted CH2, etc.; Y and Z are independently selected from N, (un)substituted CH, etc.; R1 = H, (un)substituted alk(en)yl, (hetero)aryl, cycloalkyl, etc.; R2 and R3 are independently selected from H, halogen, NO2, CN, (un)substituted alk(en)yl, etc.; R4 is H, (un)substituted alk(en)yl, CN, C(O)-alkyl, O-alkyl, etc.], their enantiomers, diastereomers, and pharmaceutically-acceptable salts, useful as anti-inflammatory agents. Compds. I were tested in an H1-HeLa adhesion assay and in a HUVEC (human umbilical vein endothelial cells) adhesion assay (no biol. data). For instance, benzimidazole derivative II was prepared via intramol. heterocyclization of the obtained urea derivative III, and N-acetylation of the obtained benzimidazole derivative IV (no yield data).

IT **681261-14-3P 681261-15-4P 681261-21-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of benzimidazolone derivs. useful as

CN 2H-Benzimidazol-2-one, 1-(3,5-dichlorophenyl)-1,3,3a,4,5,6-hexahydro-3-methyl-3a-[[4-(5-pyrimidinyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

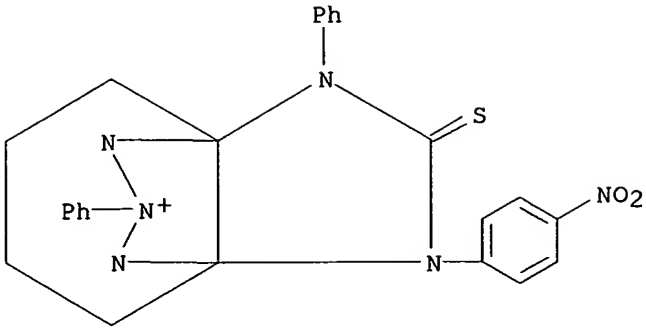


L35 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:42768 CAPLUS
DOCUMENT NUMBER: 128:127968
TITLE: Competitive reactivity of the aryl isothiocyanate dipolarophile at N:C versus C:S with nucleophilic 1,3-dipoles: a combined experimental and theoretical study. The reactions of substituted 1,2,3-triazolium-1-aminide 1,3-dipoles with aryl isothiocyanates: new tricyclic thiazolo[4,5-d][1,2,3]triazoles
AUTHOR(S): Butler, Richard N.; Grogan, Denise C.; McDonald, Peter D.; Burke, Luke A.
CORPORATE SOURCE: Chemistry Department, University College Galway, Ire.
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (24), 3587-3590
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

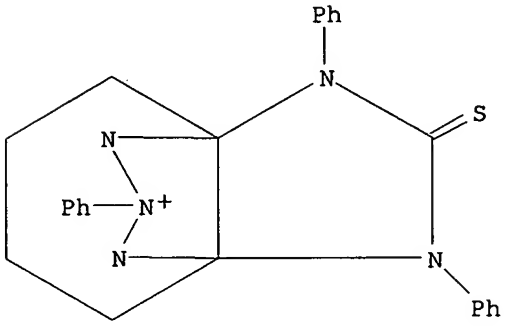
AB Substituted 1,2,3-triazolium-1-aminide 1,3-dipoles react with aryl isothiocyanates at both the N:C and C:S sites to give mixts. of substituted imidazolo[4,5-d][1,2,3]triazoles and new thiazolo[4,5-d][1,2,3]triazoles including tricyclic derivs. with the C-3a and C-6a bridgeheads linked via (CH2)4 and phenanthro groups. The product distribution is controlled by the para-substituent of the aryl isothiocyanate. Theor. calcns., 3-21G* and 6-31G*, suggest that linear triple bonded canonical forms of the aryl isothiocyanate system play a key role in the ambident reactivity of these systems.

IT **144511-37-5P 144511-38-6P 202125-87-9P 202125-89-1P 202125-91-5P 202125-93-7P 202125-97-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(reactions of substituted 1,2,3-triazolium-1-aminide 1,3-dipoles with aryl isothiocyanates)

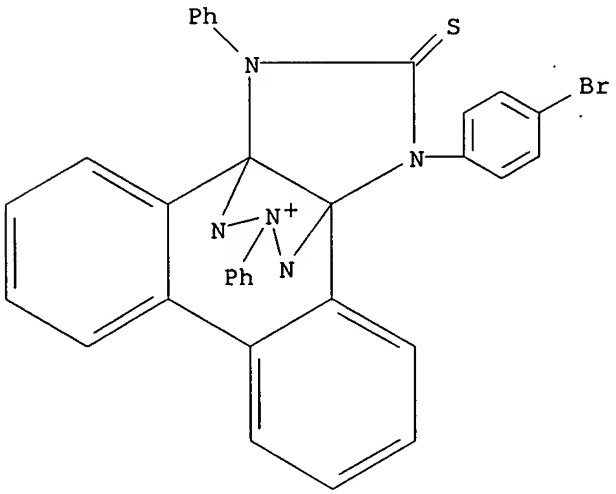
RN 144511-37-5 CAPLUS
CN 3a,7a-(Iminomethanimino)-1H-benzotriazolium, 4,5,6,7-tetrahydro-8-(4-nitrophenyl)-2,10-diphenyl-9-thioxo-, inner salt (9CI) (CA INDEX NAME)



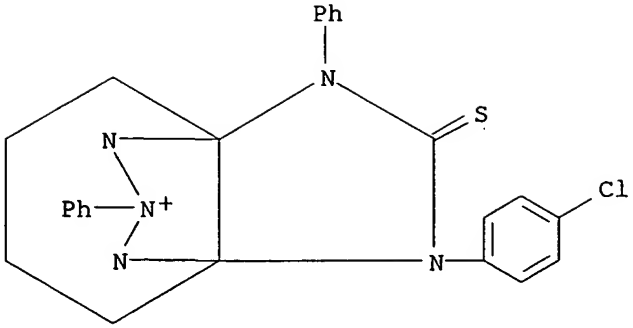
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-38-6 CAPLUS
CN 3a,7a-(Iminomethanimino)-1H-benzotriazolium, 4,5,6,7-tetrahydro-2,8,10-triphenyl-9-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 202125-87-9 CAPLUS
CN 3a,11b-(Iminomethanimino)-1H-phenanthro[9,10-d]triazolium, 12-(4-bromophenyl)-2,14-diphenyl-13-thioxo-, inner salt (9CI) (CA INDEX NAME)

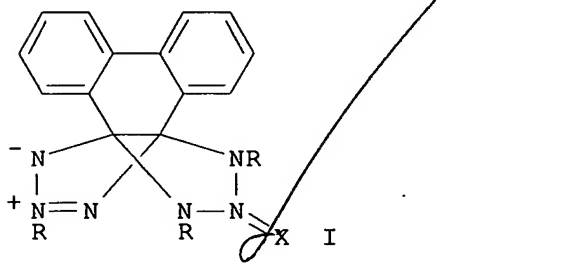


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 202125-89-1 CAPLUS
CN 3a,11b-(Iminomethanimino)-1H-phenanthro[9,10-d]triazolium, 12-(4-nitrophenyl)-2,14-diphenyl-13-thioxo-, inner salt (9CI) (CA INDEX NAME)



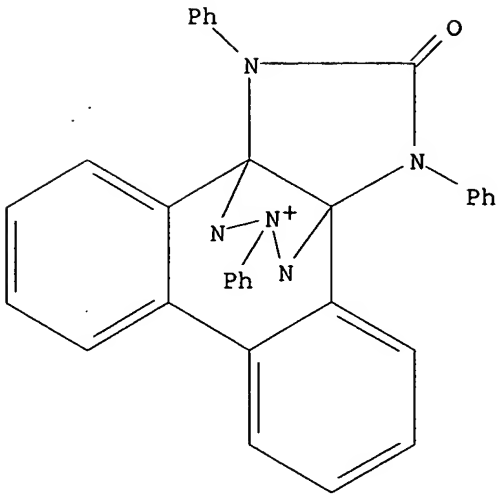
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:418477 CAPLUS
DOCUMENT NUMBER: 125:221799
TITLE: Tricyclic phenanthrene systems: substituted phenanthro[9,10-e]-1,2,3-triazines and fused phenanthroazolo-1,2,3-triazoles from cycloaddition-rearrangement sequences of 9,10-bisarylazophenanthrenes with 2π-dipolarophiles. Azolium 1,3-dipoles
AUTHOR(S): Butler, Richard N.; Lysaght, Fiona A.; McDonald, Peter D.; Pyne, Carmel S.; McArdle, Patrick; Cunningham, Desmond
CORPORATE SOURCE: Chem. Dep., Univ. College, Galway, Ire.
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1996), (13), 1623-1627
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:221799
GI



I

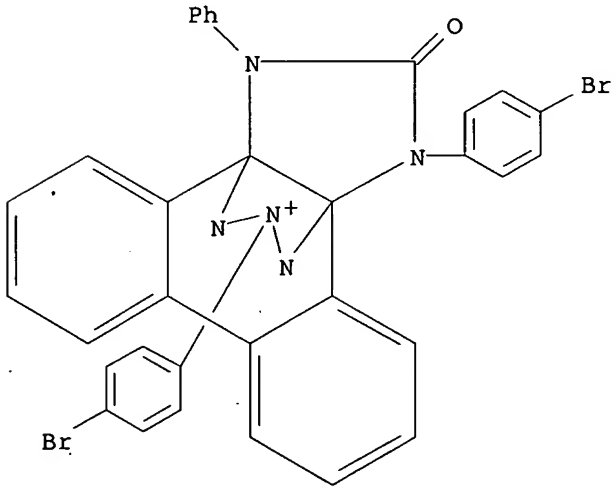
AB A range of new fused ring systems based on phenanthrene was obtained from cycloaddn.-rearrangement reactions of 9,10-bisarylazophenanthrenes with alkyne and alkene dipolarophiles. These new rings include substituted phenanthro[9,10-e]-1,2,3-triazines and tricyclic systems, e.g., trisubstituted 3a,6a-(biphen-2,2'-yl)hexahydropyrrolo[2,3-d]-1,2,3-triazoles and substituted 3a,6a-(biphen-2,2'-yl)-hexahydroimidazo[4,5-d]-1,2,3-triazoles. X-Ray crystal structures are reported on 2-(p-bromophenyl)-4-methoxycarbonyl-4-(p-bromophenyliminomethoxalyl)-3,4-



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 181054-14-8 CAPLUS

CN 3a,11b-(Iminomethanimino)-1H-phenanthro[9,10-d]triazolium, 2,12-bis(4-bromophenyl)-13-oxo-14-phenyl-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L35 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:651292 CAPLUS

DOCUMENT NUMBER: 117:251292

TITLE: Substituted tetrahydroimidazo[4,5-d][1,2,3]triazoles and hexahydrobutanoimidazo[4,5-d][1,2,3]triazoles from the reaction of 1,2,3-triazolium-1-imides with aryl isocyanates and isothiocyanates. Azolium 1,3-dipoles

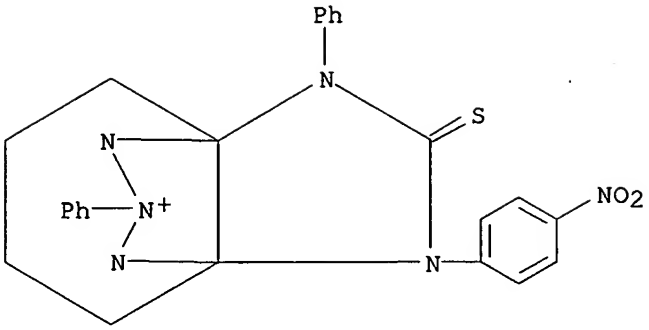
AUTHOR(S): Butler, Richard; Colleran, David M.

CORPORATE SOURCE: Chem. Dep., Univ. Coll., Galway, Ire.

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1992), (17), 2159-61
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

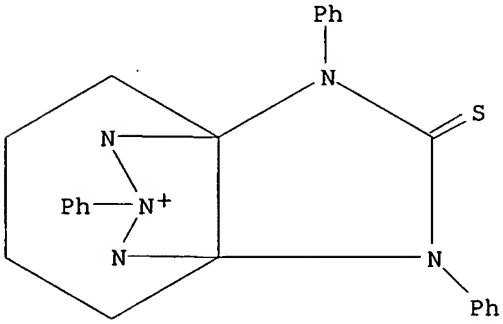
LANGUAGE: English



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 144511-38-6 CAPLUS

CN 3a,7a-(Iminomethanimino)-1H-benzotriazolium, 4,5,6,7-tetrahydro-2,8,10-triphenyl-9-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L35 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1982:68857 CAPLUS

DOCUMENT NUMBER: 96:68857

TITLE: 2',3',4',9'-Tetrahydrospiro[cyclohexane-1,1'-(1H)pyrido[3,4-b]indol]-2-ones and their transformations into 2,3,4,4a,5,6,9,14-octahydro-4a-hydroxy-1H,8H-pyrido[3,4-b:2,1-i']diindole-5-carbonitriles and 5-substituted 2,3,4,4a,9,14-hexahydro-4a-hydroxy-1H,8H-indolo[2',3':3,4]pyrido[1,2-c]benzimidazol-6-(5H)ones

AUTHOR(S): Bobowski, George

CORPORATE SOURCE: Warner-Lambert/Parke-Davis Pharm. Res. Div., Ann Arbor, MI, 48105, USA

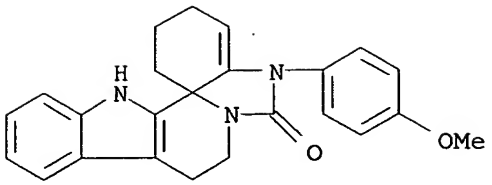
SOURCE: Journal of Heterocyclic Chemistry (1981), 18(6), 1179-87
CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

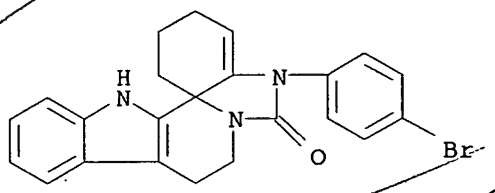
LANGUAGE: English

OTHER SOURCE(S): CASREACT 96:68857

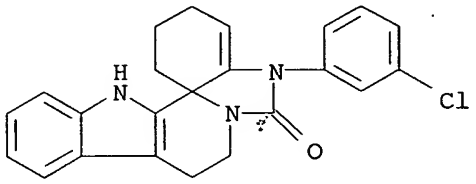
AB 1H-Indole-3-ethanamine derivs. were condensed with 1,2-cyclohexanedione and the resulting 2-[[2-(1H-indol-3-yl)ethyl]imino]cyclohexanones were converted into 2',3',4',9'-tetrahydrospiro[cyclohexane-1,1'-(1H)pyrido[3,4-b]indol]-2-ones (I) under Pictet-Spengler reaction conditions. The reaction of I with acrylonitrile gave 2,3,4,4a,5,6,9,14-octahydro-4a-hydroxy-1H,8H-pyrido[3,4-b:2,1-i']diindole-5-carbonitriles. Treatment of I with alkyl and aryl isocyanates at room temperature gave 5-substituted-2,3,4,4a,9,14-hexahydro-4a-hydroxy.1H,8H-indolo[2',3':3,4]pyrido[1,2-c]benzimidazol-6(5H)-ones. Dehydration of the latter gave



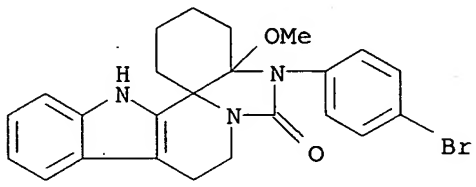
RN 80616-18-8 CAPLUS
CN 2H,4H-Indolo[2',3':3,4]pyrido[1,2-c]benzimidazol-2-one,
1-(4-bromophenyl)-1,5,10,11,12,13-hexahydro- (9CI) (CA INDEX NAME)



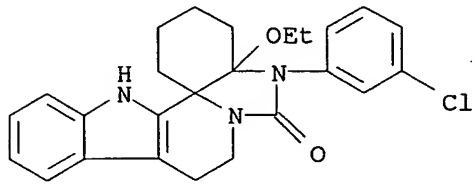
RN 80616-19-9 CAPLUS
CN 2H,4H-Indolo[2',3':3,4]pyrido[1,2-c]benzimidazol-2-one,
1-(3-chlorophenyl)-1,5,10,11,12,13-hexahydro- (9CI) (CA INDEX NAME)



RN 80616-20-2 CAPLUS
CN 2H,4H-Indolo[2',3':3,4]pyrido[1,2-c]benzimidazol-2-one,
1-(4-bromophenyl)-1,5,10,11,12,13,14,14a-octahydro-14a-methoxy- (9CI) (CA INDEX NAME)



RN 80616-21-3 CAPLUS
CN 2H,4H-Indolo[2',3':3,4]pyrido[1,2-c]benzimidazol-2-one,
1-(3-chlorophenyl)-14a-ethoxy-1,5,10,11,12,13,14,14a-octahydro- (9CI) (CA INDEX NAME)

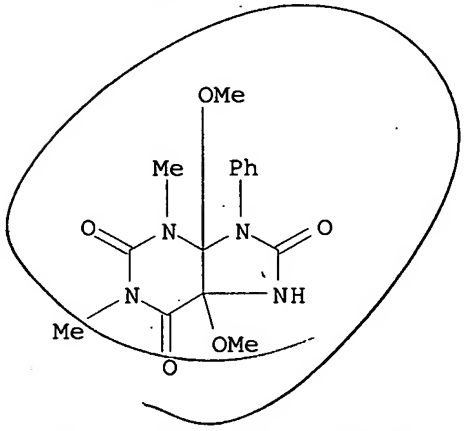


L35 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1969:77916 CAPLUS
DOCUMENT NUMBER: 70:77916
TITLE: Photoinduced reactions. XXIV. Photosensitized oxygenation of hydroxylated 9-phenylpurines
AUTHOR(S): Matsuura, Teruo; Saito, Isao
CORPORATE SOURCE: Kyoto Univ., Kyoto, Japan
SOURCE: Tetrahedron (1969), 25(3), 541-7
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 70:77916

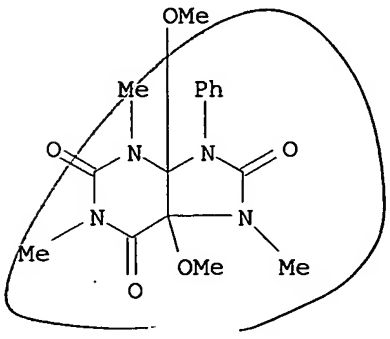
AB Photosensitized oxygenation of 1,3-dimethyl-9-phenylxanthine and 9-phenylxanthine in methanol in the presence of Rose Bengal gave as the major products the corresponding 4,5-dihydro-4,5-dimethoxyuric acid (I) and its 1,3-dimethyl derivative (II), resp. Under similar conditions, 1,3-dimethyl-9-phenyluric acid (III) and 9-phenyluric acid yielded I and II, resp. In the case of III, 1,3-dimethyl-4-hydroxy-5-methoxy-9-phenyluric acid was also obtained. Possible mechanisms involving peroxide intermediates, a 4,8-endo-peroxide and a 4-hydroperoxide, are discussed.

IT **22305-91-5P 22305-93-7P 22305-94-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

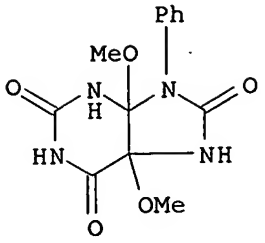
RN 22305-91-5 CAPLUS
CN Uric acid, dihydro-4,5-dimethoxy-1,3-dimethyl-9-phenyl- (8CI) (CA INDEX NAME)



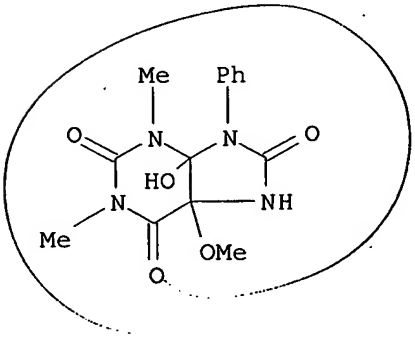
RN 22305-93-7 CAPLUS
CN Uric acid, dihydro-4,5-dimethoxy-1,3,7-trimethyl-9-phenyl- (8CI) (CA INDEX NAME)



RN 22305-94-8 CAPLUS
CN Uric acid, dihydro-4,5-dimethoxy-9-phenyl- (8CI) (CA INDEX NAME)



L35 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1968:467330 CAPLUS
DOCUMENT NUMBER: 69:67330
TITLE: Photo-induced reactions. XV. The nature of peroxide intermediates in the photosensitized oxygenation of purine derivatives
AUTHOR(S): Matsuura, Teruo; Saito, Isao
CORPORATE SOURCE: Kyoto Univ., Kyoto, Japan
SOURCE: Tetrahedron Letters (1968), (29), 3273-6
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Photooxygenation of I (R = R1 = H, R2 = Ph), I (R = R1 = Me, R2 = Ph), II (R = R1 = R3 = H, R2 = Ph), II (R = R1 = Me, R2 = Ph, R3 = H) (III), and II (R = R1 = R2 = R3 = Me) (IV) in MeOH in the presence of rose bengal gave V(R = R1 = R3 = H, R2 = Ph, R4 = Me) (VI) (58%), V(R = R1 = Me, R2 = Ph, R3 = R4 = Me) (VII) (23.3%), VI (46%), VII (2.1%), and V (R = R1 = R2 = R3 = R4 = Me) (35%), resp. III and IV also gave 11.4% V(R = R1 = Me, R2 = Ph, R3 = R4 = H) and 5% allocaffic acid, resp. Photosensitized oxygenation of IV in CHCl3 in the presence of methylene blue gave 18% VIII (R = Me) and II (R = Et, R1 = R2 = R3 = Me) gave 12% VIII (R = Et), 8% N,N'-dimethylparabanic acid and 22% IX. VI and VII are formed from the corresponding I via an endo-peroxide intermediate, while VI, VII, and V(R = R1 = R2 = R3 = R4 = Me) are formed from the corresponding II via the zwitterion peroxide X.
IT **19983-95-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19983-95-0 CAPLUS
CN Uric acid, 4,5-dihydro-4-hydroxy-5-methoxy-1,3-dimethyl-9-phenyl- (8CI) (CA INDEX NAME)



=> fil reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	37.28	1275.92

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-5.11	-33.58

FILE 'REGISTRY' ENTERED AT 09:42:43 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 APR 2005 HIGHEST RN 847818-85-3
DICTIONARY FILE UPDATES: 1 APR 2005 HIGHEST RN 847818-85-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

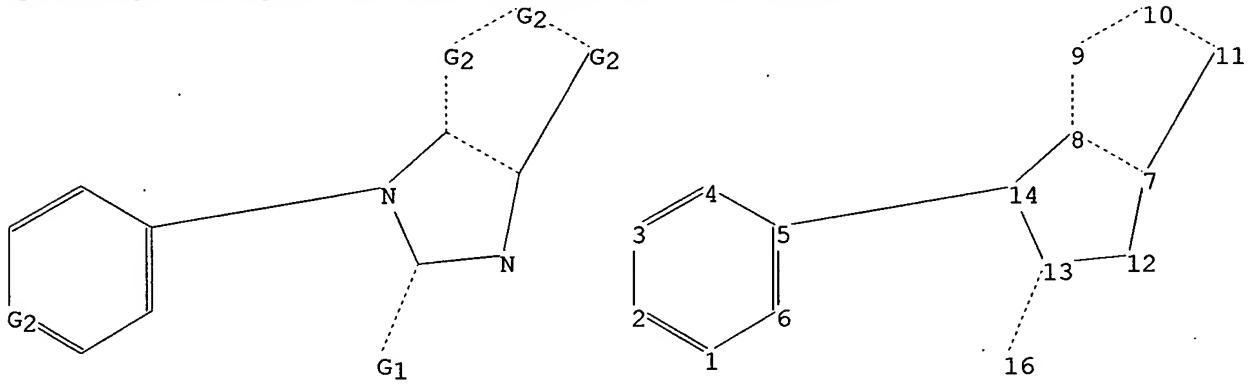
****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Revise search

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10681924g.str



chain nodes :
16
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14
chain bonds :
5-14 13-16
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-11 8-9 8-14 9-10 10-11 12-13 13-14

exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-14 7-8 7-12 7-11 8-9 8-14 9-10 10-11 12-13
13-14 13-16

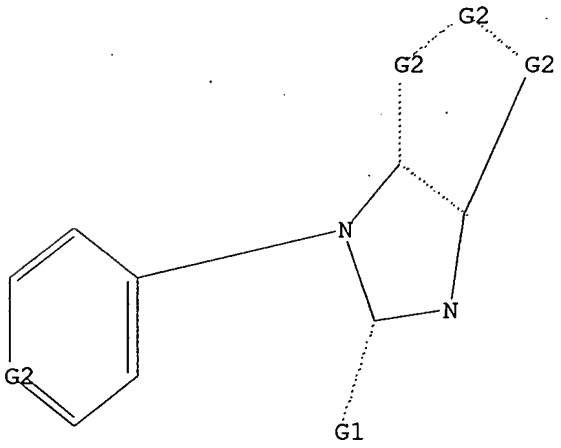
G1:O,S

G2:C,N

Hydrogen count :
7:= exact 0
Connectivity :
7:4 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 16:CLASS

L36 STRUCTURE UPLOADED

=> d
L36 HAS NO ANSWERS
L36 STR



G1 O,S
G2 C,N

Structure attributes must be viewed using STN Express query preparation.

=> s L36 full
FULL SEARCH INITIATED 09:43:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 34288 TO ITERATE

100.0% PROCESSED 34288 ITERATIONS 64 ANSWERS
SEARCH TIME: 00.00.01

L37 64 SEA SSS FUL L36

=> fil caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	1437.25

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION

CA SUBSCRIBER PRICE 0.00 -33.58

FILE 'CAPLUS' ENTERED AT 09:43:19 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 4 Apr 2005 VOL 142 ISS 15
FILE LAST UPDATED: 3 Apr 2005 (20050403/ED)

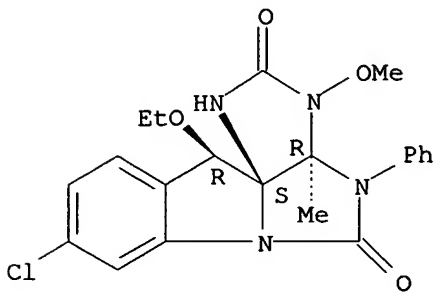
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L37
L38 14 L37

=> d ibib abs hitstr 1-14

L38 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:1005699 CAPLUS
DOCUMENT NUMBER: 142:288078
TITLE: Crystal structure of 6-chloro-2-ethoxy-13-methoxy-12-methyl-11-phenyl-9,11,13,15-tetraazatetracyclo[7.6.0.01,12.03,8]pentadeca-3,5,7-triene-10,14-dione
AUTHOR(S): Seguchi, Kazuyoshi; Tanaka, Satoko; Kobayashi, Ai
CORPORATE SOURCE: School of Human Environmental Sciences, Mukogawa Women's University, Nishinoniya, 663-8558, Japan
SOURCE: X-Ray Structure Analysis Online (2004), 20(Oct.-Dec.), x147-x148
CODEN: XSAOAF
URL: http://wwwsoc.nii.ac.jp/jsac/analsci/pdfs/x-04-147.pdf
PUBLISHER: Japan Society for Analytical Chemistry
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
AB The title compound was synthesized and its structure characterized by x-ray diffraction. This compound crystallizes in monoclinic space group P21/n with a 7.3400(4), b 11.4484(5), c 23.342(1) Å, β 91.5490(8)°, and Z = 4; the final residual factor is R = 0.048 for 4152 reflections. The stereochem. between the ethoxy group in the indoline ring and the cyclic urea having the N-methoxy group is cis-configuration.
IT **847401-21-2P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
RN 847401-21-2 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.



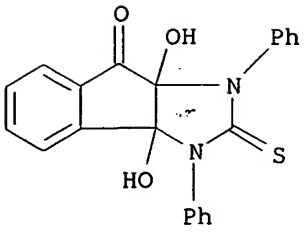
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:740922 CAPLUS
DOCUMENT NUMBER: 139:365000
TITLE: Waste-free and facile solid-state protection of diamines, anthranilic acid, diols, and polyols with phenylboronic acid
AUTHOR(S): Kaupp, Gerd; Naimi-Jamal, M. Reza; Stepanenko, Vladimir
CORPORATE SOURCE: University of Oldenburg Fakultaet 5, Organische Chemie I, Oldenburg, 26111, Germany
SOURCE: Chemistry--A European Journal (2003), 9(17), 4156-4160
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:365000

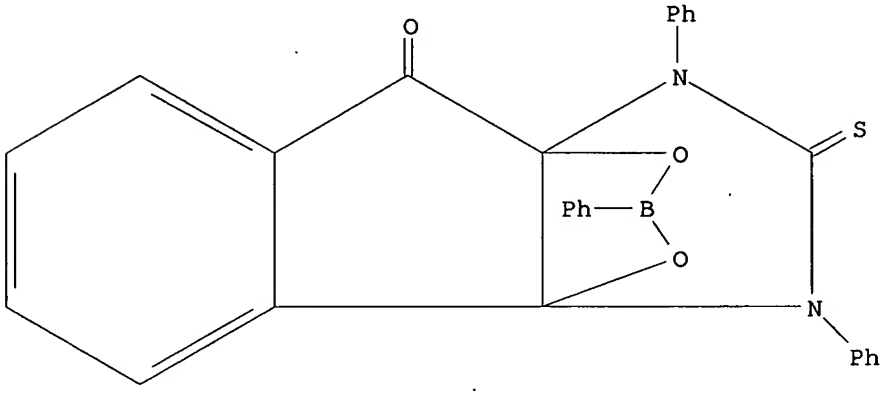
AB Phenylboronic acid (2) reacts quant. by ball-milling in the solid state with o-phenylendiamine, 1,8-diaminonaphthalene, anthranilic acid, pyrocatechol, pyrogallol, pinacol, bicyclic cis-diols, mannitol, and inositol to form the five- or six-membered cyclic phenylboronic amides or esters. Catalysts or other auxiliaries are strictly excluded as they are not required and would have to be removed after the reactions. These varied model reactions provide pure protected products without the necessity of further purifying workup and the potential for protection chemical is demonstrated. Some of the reactions can also be quant. performed if stoichiometric mixts. of the reactants are co-ground or co-milled and heated to appropriate temps. either below the eutectics or above the m.ps. The temps. are much higher in the latter case. Similar reactions in solution suffer from <100% yield of the mostly sensitive compds. that are difficult to purify and thus create much waste. The hydrolysis (deprotection) conditions of the products are rather mild in most cases. Therefore, this particularly easy access to heteroboroles, heteroborolanes, heteroborinones, heteroborines, and heteroborinines is highly valuable for their more frequent use in protective syntheses.

IT **301157-54-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(waste-free and facile solid-state reaction of diamines, anthranilic acid, diols, and polyols with phenylboronic acid to give five- and six-membered cyclic phenylboronic amides and esters)

RN 301157-54-0 CAPLUS
CN Indeno[1,2-d]imidazol-8(1H)-one, 2,3,3a,8a-tetrahydro-3a,8a-dihydroxy-1,3-diphenyl-2-thioxo- (9CI) (CA INDEX NAME)



IT **622410-30-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(waste-free and facile solid-state reaction of diamines, anthranilic acid, diols, and polyols with phenylboronic acid to give five- and six-membered cyclic phenylboronic amides and esters)
RN 622410-30-4 CAPLUS
CN 1H,8H-3a,8a-(Epoxyborylenoxy)indeno[1,2-d]imidazol-8-one, 2,3-dihydro-1,3,10-triphenyl-2-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

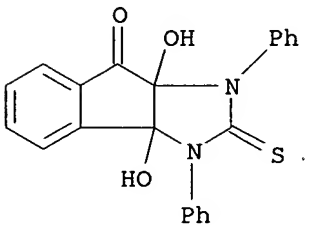
L38 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:140306 CAPLUS
DOCUMENT NUMBER: 137:20356
TITLE: Quantitative reaction cascades of ninhydrin in the solid state
AUTHOR(S): Kaupp, Gerd; Naimi-Jamal, M. Reza; Schmeyers, Jens
CORPORATE SOURCE: FB Chemie, Organische Chemie 1, University of Oldenburg, Oldenburg, 26111, Germany
SOURCE: Chemistry--A European Journal (2002), 8(3), 594-600
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:20356
AB Crystalline ninhydrin (I) undergoes waste-free solid-state cascade reactions with dimedone, L-proline, three o-phenylenediamines, o-mercaptoaniline, two ureas, three thioureas, and Me 3-aminocrotonate. The yields are quant. and give pure crystalline products without workup just by milling stoichiometric mixts. of the crystalline reagents. The structures of the new and the previously obtained products with lower yields from solns. are established or confirmed by spectroscopic data and d. functional calcns. at the B3LYP/6-31G* level. The success of 3- and 4-cascade reactions in the crystal without melting is unusual and of unmatched atom economy.

They are mechanistically investigated with atomic force microscopy techniques (AFM) on six different faces of I when o-phenylenediamine was the reagent (substitution, elimination, cyclization, elimination) and interpreted on the basis of known crystal structure data. Strict correlations to the crystal packings are observed The characteristic surface features grow to μm heights in some cases at distances of 0.5 mm from the contact edge of the reacting crystals. The waste-free and easy syntheses of highly functionalized (C=O; O-H; C=N) heterocycles or of a tetraketone are also of interest for synthetic use.

IT **301157-54-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(quant. reaction cascades of ninhydrin in the solid state)

RN 301157-54-0 CAPLUS

CN Indeno[1,2-d]imidazol-8(1H)-one, 2,3,3a,8a-tetrahydro-3a,8a-dihydroxy-1,3-diphenyl-2-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:591739 CAPLUS

DOCUMENT NUMBER: 133:296418

TITLE: Synthesis and anticonvulsant activity of some 2,4-disubstituted-2,4-benzodiazocine-1,3,5,6-tetrones, 1-mono and 1,3-disubstituted indenoimidazoles and 2-substituted imidazoisoindoles

AUTHOR(S): Sarra, Joseph D.; Stephani, Ralph A.

CORPORATE SOURCE: Department of Chemistry, C.W. Post Campus of Long Island University, Brookville, NY, 11548, USA

SOURCE: Medicinal Chemistry Research (2000), 10(2), 81-91
CODEN: MCREEB; ISSN: 1054-2523

PUBLISHER: Birkhaeuser Boston

DOCUMENT TYPE: Journal

LANGUAGE: English

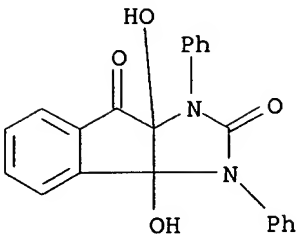
OTHER SOURCE(S): CASREACT 133:296418

AB 1-Mono and 1,3- disubstituted indeno[1,2-d] imidazolones were synthesized by reaction of appropriately mono- and disubstituted ureas with ninhydrin, in aqueous alc. and heat. Oxidation of these with Na metaperiodate formed the corresponding imidazo[5,1-a]isoindoles and benzodiazocinetetrones, resp. Compds. were evaluated for anticonvulsant activity by their ability to protect against pentylenetetrazole-induced convulsions, in mice. Indenoimidazoles and imidazoisoindoles had no significant anticonvulsant activity, but the latter possessed acute lethalities. Benzodiazocinetetrones exhibited significant anticonvulsant activities, with no acute toxicities observed

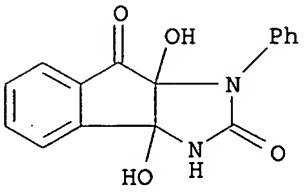
IT **58137-72-7P 301157-42-6P 301157-54-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation from ninhydrin and ureas)

RN 58137-72-7 CAPLUS

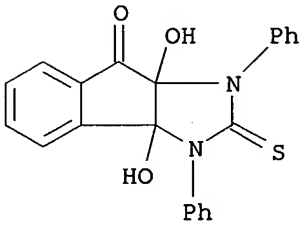
CN Indeno[1,2-d]imidazole-2,8-dione, 1,3,3a,8a-tetrahydro-3a,8a-dihydroxy-1,3-diphenyl- (9CI) (CA INDEX NAME)



RN 301157-42-6 CAPLUS
CN Indeno[1,2-d]imidazole-2,8-dione, 1,3,3a,8a-tetrahydro-3a,8a-dihydroxy-1-phenyl- (9CI) (CA INDEX NAME)



RN 301157-54-0 CAPLUS
CN Indeno[1,2-d]imidazol-8(1H)-one, 2,3,3a,8a-tetrahydro-3a,8a-dihydroxy-1,3-diphenyl-2-thioxo- (9CI) (CA INDEX NAME)

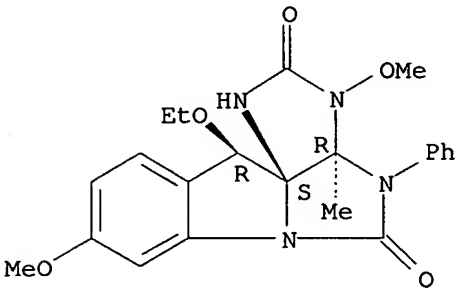


REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:515429 CAPLUS
DOCUMENT NUMBER: 131:207174
TITLE: Crystal structure of 2-ethoxy-6,13-dimethoxy-12-methyl-11-phenyl-9,11,13,15-tetraazatetracyclo[7.6.0.01,12.03,8]pentadeca-3,4,6-triene-10,14-dione
AUTHOR(S): Tanaka, Satoko; Kato, Katsuya; Kimoto, Hiroshi; Seguchi, Kazuyoshi
CORPORATE SOURCE: National Industrial Research Institute of Nagoya, Nagoya, 462-8510, Japan
SOURCE: Analytical Sciences (1999), 15(8), 817-818
CODEN: ANSCEN; ISSN: 0910-6340
PUBLISHER: Japan Society for Analytical Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The title compound is monoclinic, space group P21/c, with a 7.775(3), b 31.778(3), c 8.806(3) Å, β 103.78(2)°; dc = 1.334 for Z = 4, R = 0.049 and Rw = 0.080 for 2484 reflections. Atomic coordinates are given. Dihedral angles and ring conformation are discussed.
IT **240813-14-3**

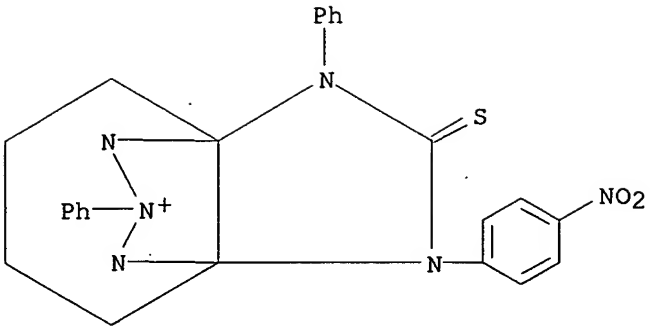
RL: PRP (Properties)
(crystal structure of)
RN 240813-14-3 CAPLUS
CN 11H-Imidazo[4',5':4,5]imidazo[1,5-a]indole-2,5(1H,3H)-dione, 11-ethoxy-3a,4-dihydro-3,8-dimethoxy-3a-methyl-4-phenyl-, (3aR,11R,11aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

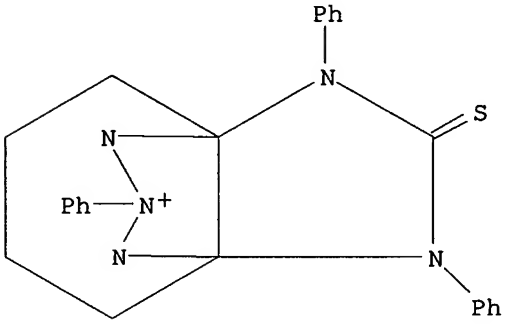


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:42768 CAPLUS
DOCUMENT NUMBER: 128:127968
TITLE: Competitive reactivity of the aryl isothiocyanate dipolarophile at N:C versus C:S with nucleophilic 1,3-dipoles: a combined experimental and theoretical study. The reactions of substituted 1,2,3-triazolium-1-aminide 1,3-dipoles with aryl isothiocyanates: new tricyclic thiazolo[4,5-d][1,2,3]triazoles
AUTHOR(S): Butler, Richard N.; Grogan, Denise C.; McDonald, Peter D.; Burke, Luke A.
CORPORATE SOURCE: Chemistry Department, University College Galway, Ire.
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (24), 3587-3590
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Substituted 1,2,3-triazolium-1-aminide 1,3-dipoles react with aryl isothiocyanates at both the N:C and C:S sites to give mixts. of substituted imidazolo[4,5-d][1,2,3]triazoles and new thiazolo[4,5-d][1,2,3]triazoles including tricyclic derivs. with the C-3a and C-6a bridgeheads linked via (CH2)4 and phenanthro groups. The product distribution is controlled by the para-substituent of the aryl isothiocyanate. Theor. calcns., 3-21G* and 6-31G*, suggest that linear triple bonded canonical forms of the aryl isothiocyanate system play a key role in the ambident reactivity of these systems.
IT **144511-37-5P 144511-38-6P 202125-81-3P 202125-83-5P 202125-85-7P 202125-87-9P 202125-89-1P 202125-91-5P 202125-93-7P 202125-97-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(reactions of substituted 1,2,3-triazolium-1-aminide 1,3-dipoles with aryl isothiocyanates)
RN 144511-37-5 CAPLUS
CN 3a,7a-(Iminomethanimino)-1H-benzotriazolium, 4,5,6,7-tetrahydro-8-(4-nitrophenyl)-2,10-diphenyl-9-thioxo-, inner salt (9CI) (CA INDEX NAME)

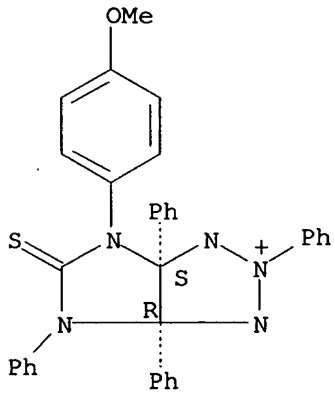


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-38-6 CAPLUS
CN 3a,7a-(Iminomethanimino)-1H-benzotriazolium, 4,5,6,7-tetrahydro-2,8,10-triphenyl-9-thioxo-, inner salt (9CI) (CA INDEX NAME)



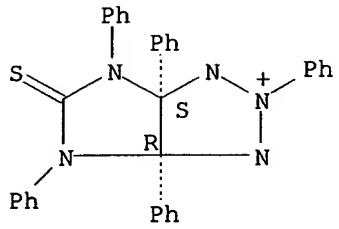
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 202125-81-3 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-4-(4-methoxyphenyl)-2,3a,6,6a-tetraphenyl-5-thioxo-, inner salt, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



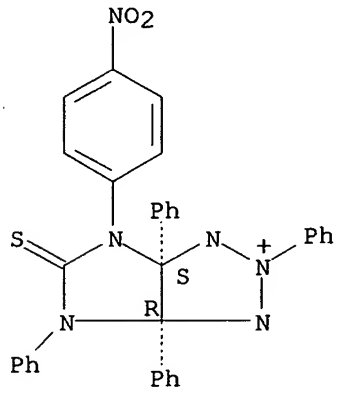
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 202125-83-5 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-2,3a,4,6,6a-pentaphenyl-5-thioxo-, inner salt, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

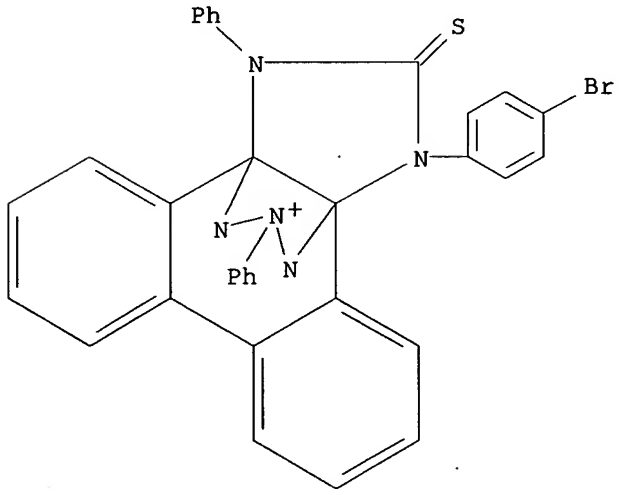


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 202125-85-7 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-4-(4-nitrophenyl)-2,3a,6,6a-tetraphenyl-5-thioxo-, inner salt, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

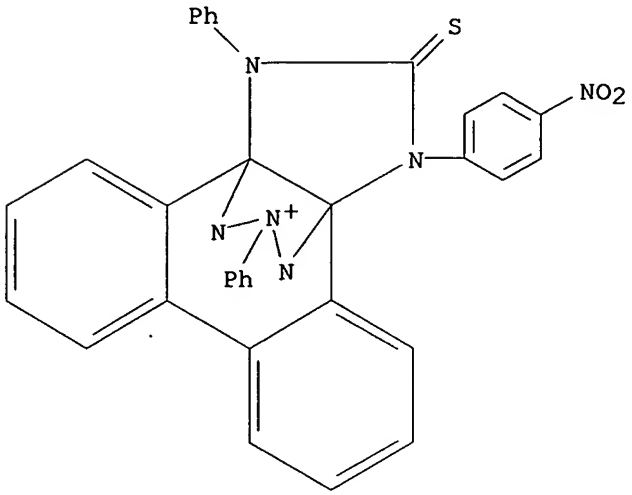


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 202125-87-9 CAPLUS
CN 3a,11b-(Iminomethanimino)-1H-phenanthro[9,10-d]triazolium, 12-(4-bromophenyl)-2,14-diphenyl-13-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 202125-89-1 CAPLUS

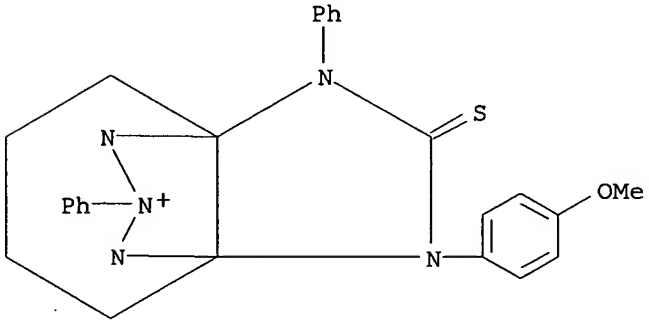
CN 3a,11b-(Iminomethanimino)-1H-phenanthro[9,10-d]triazolium, 12-(4-nitrophenyl)-2,14-diphenyl-13-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 202125-91-5 CAPLUS

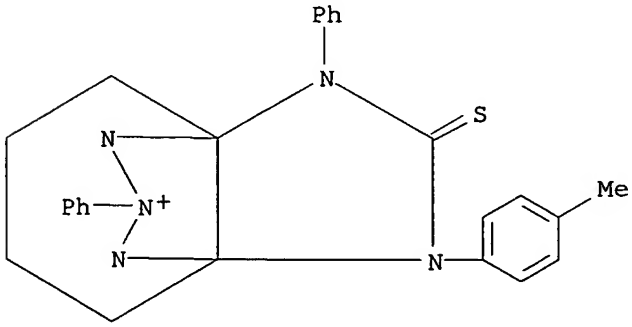
CN 3a,7a-(Iminomethanimino)-1H-benzotriazolium, 4,5,6,7-tetrahydro-8-(4-methoxyphenyl)-2,10-diphenyl-9-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

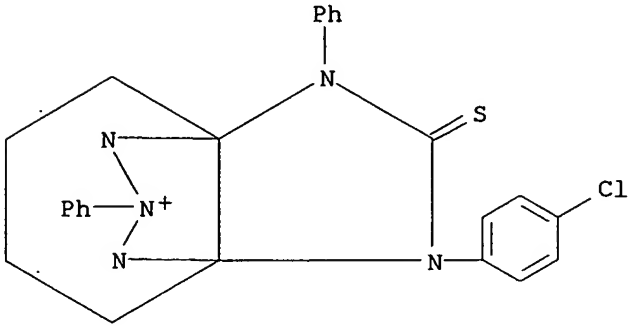
RN 202125-93-7 CAPLUS

CN 3a,7a-(Iminomethanimino)-1H-benzotriazolium, 4,5,6,7-tetrahydro-8-(4-methylphenyl)-2,10-diphenyl-9-thioxo-, inner salt (9CI) (CA INDEX NAME)



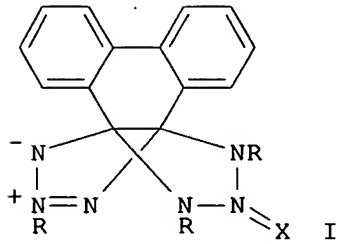
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 202125-97-1 CAPLUS
CN 3a,7a-(Iminomethanimino)-1H-benzotriazolium, 8-(4-chlorophenyl)-4,5,6,7-tetrahydro-2,10-diphenyl-9-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:418477 CAPLUS
DOCUMENT NUMBER: 125:221799
TITLE: Tricyclic phenanthrene systems: substituted phenanthro[9,10-e]-1,2,3-triazines and fused phenanthroazolo-1,2,3-triazoles from cycloaddition-rearrangement sequences of 9,10-bisarylazophenanthrenes with 2π-dipolarophiles. Azolium 1,3-dipoles
AUTHOR(S): Butler, Richard N.; Lysaght, Fiona A.; McDonald, Peter D.; Pyne, Carmel S.; McArdle, Patrick; Cunningham, Desmond
CORPORATE SOURCE: Chem. Dep., Univ. College, Galway, Ire.
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1996), (13), 1623-1627
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:221799
GI



I

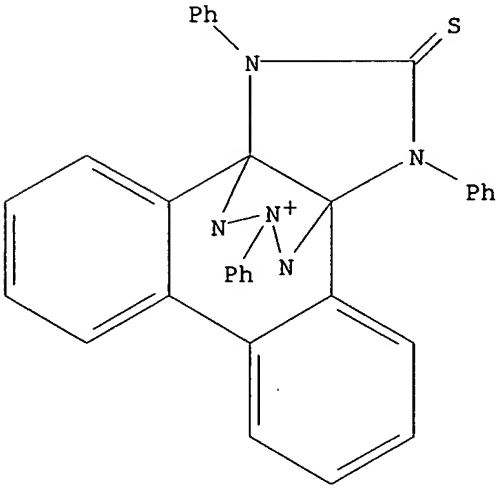
AB A range of new fused ring systems based on phenanthrene was obtained from cycloaddn.-rearrangement reactions of 9,10-bisarylazophenanthrenes with alkyne and alkene dipolarophiles. These new rings include substituted phenanthro[9,10-e]-1,2,3-triazines and tricyclic systems, e.g., trisubstituted 3a,6a-(biphen-2,2'-yl)hexahydropyrrolo[2,3-d]-1,2,3-

triazoles and substituted 3a,6a-(biphen-2,2'-yl)-hexahydroimidazo[4,5-d]-1,2,3-triazoles. X-Ray crystal structures are reported on 2-(p-bromophenyl)-4-methoxycarbonyl-4-(p-bromophenyliminomethoxalyl)-3,4-dihydrophenanthro[9,10-e]-1,2,3-triazin-2-ium-3-ide and 2,4-diphenyl-3a,6a-(biphen-2,2'-yl)-5,6-endo-dicarboxy-N-phenylimido-1,3a,4,5,6,6a-hexahydropyrrolo[2,3-d]-1,2,3-triazol-2-ium-1-ide. Example compds. thus prepared are thephenanthrotriazinium compds. I (X = O, S, R = substituted phenyl).

IT **181054-09-1P 181054-10-4P 181054-11-5P**
181054-12-6P 181054-13-7P 181054-14-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of phenanthrotriazines and phenanthroazolotriazoles by cycloaddn. and rearrangement arylazophenanthrenes with dipolarophiles)

RN 181054-09-1 CAPLUS

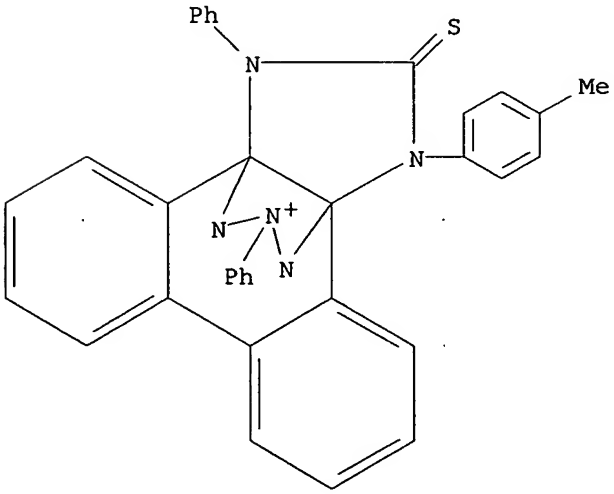
CN 3a,11b-(Iminomethanimino)-1H-phenanthro[9,10-d]triazolium, 2,12,14-triphenyl-13-thioxo-, inner salt (9CI) (CA INDEX NAME)



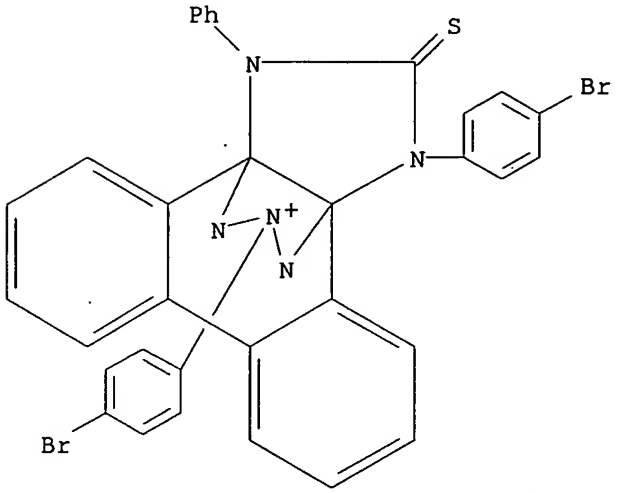
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 181054-10-4 CAPLUS

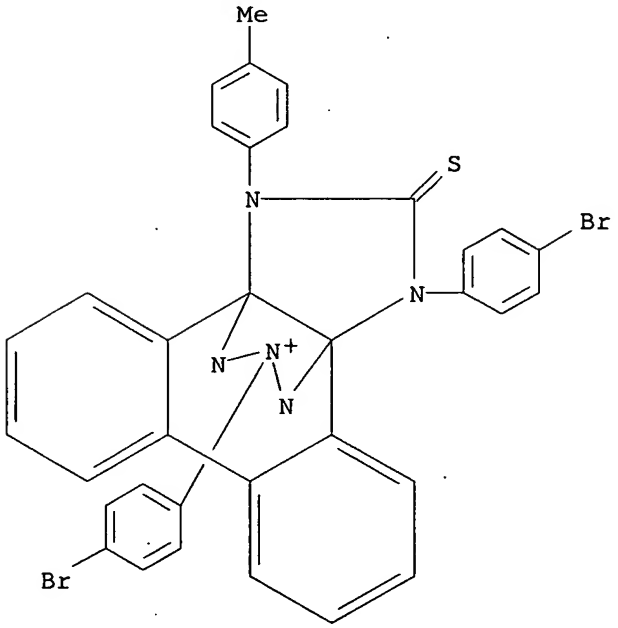
CN 3a,11b-(Iminomethanimino)-1H-phenanthro[9,10-d]triazolium, 12-(4-methylphenyl)-2,14-diphenyl-13-thioxo-, inner salt (9CI) (CA INDEX NAME)



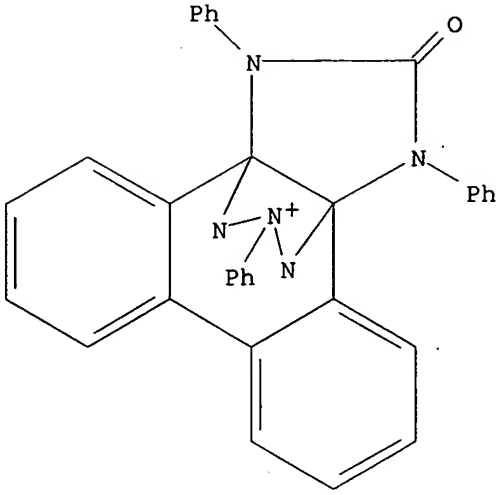
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 181054-11-5 CAPLUS
CN 3a,11b-(Iminomethanimino)-1H-phenanthro[9,10-d]triazolium, 2,12-bis(4-bromophenyl)-14-phenyl-13-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 181054-12-6 CAPLUS
CN 3a,11b-(Iminomethanimino)-1H-phenanthro[9,10-d]triazolium, 2,12-bis(4-bromophenyl)-14-(4-methylphenyl)-13-thioxo-, inner salt (9CI) (CA INDEX NAME)



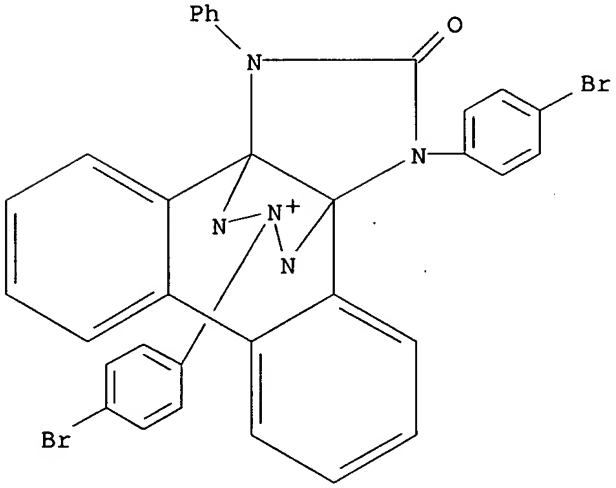
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 181054-13-7 CAPLUS
CN 3a,11b-(Iminomethanimino)-1H-phenanthro[9,10-d]triazolium, 13-oxo-2,12,14-triphenyl-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 181054-14-8 CAPLUS

CN 3a,11b-(Iminomethanimino)-1H-phenanthro[9,10-d]triazolium, 2,12-bis(4-bromophenyl)-13-oxo-14-phenyl-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L38 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:651292 CAPLUS

DOCUMENT NUMBER: 117:251292

TITLE: Substituted tetrahydroimidazo[4,5-d][1,2,3]triazoles and hexahydrobutanoimidazo[4,5-d][1,2,3]triazoles from the reaction of 1,2,3-triazolium-1-imides with aryl isocyanates and isothiocyanates. Azolium 1,3-dipoles

AUTHOR(S): Butler, Richard; Colleran, David M.

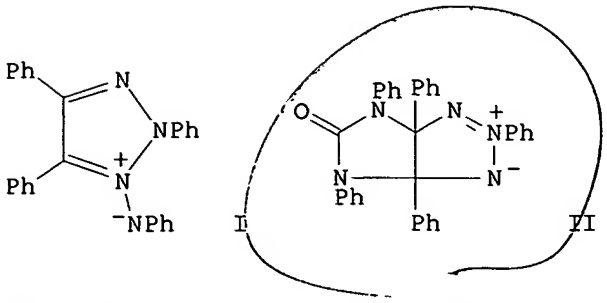
CORPORATE SOURCE: Chem. Dep., Univ. Coll., Galway, Ire.

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1992), (17), 2159-61
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

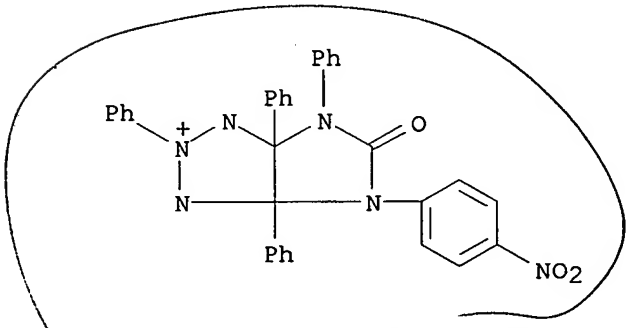


AB The reaction of aryl substituted 1,2,3-triazolium-1-imide 1,3-dipoles, e.g. I, with substituted aryl isocyanates, e.g. PhNCO, and isothiocyanates gave new ring systems based on the imidazo[4,5-c][1,2,3]triazole structure, e.g. II. With the isothiocyanates an apparent exchange of aryl groups between the dipole and recovered isothiocyanate dipolarophile sheds light on the initial intermediate in the reaction.

IT **144511-16-0P 144511-17-1P 144511-18-2P**
144511-19-3P 144511-20-6P 144511-21-7P
144511-22-8P 144511-23-9P 144511-24-0P
144511-25-1P 144511-26-2P 144511-27-3P
144511-28-4P 144511-29-5P 144511-30-8P
144511-31-9P 144511-32-0P 144511-33-1P
144511-34-2P 144511-35-3P 144511-36-4P
144511-37-5P 144511-38-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 144511-16-0 CAPLUS

CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-4-(4-nitrophenyl)-5-oxo-2,3a,6,6a-tetraphenyl-, inner salt (9CI) (CA INDEX NAME)

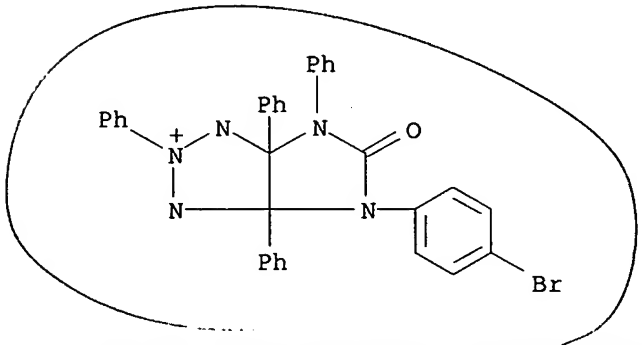


close

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 144511-17-1 CAPLUS

CN Imidazo[4,5-d]-1,2,3-triazolium, 4-(4-bromophenyl)-1,3a,4,5,6,6a-hexahydro-5-oxo-2,3a,6,6a-tetraphenyl-, inner salt (9CI) (CA INDEX NAME)



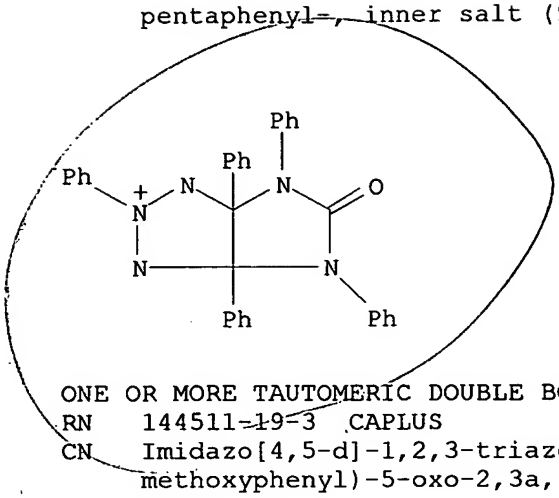
close

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

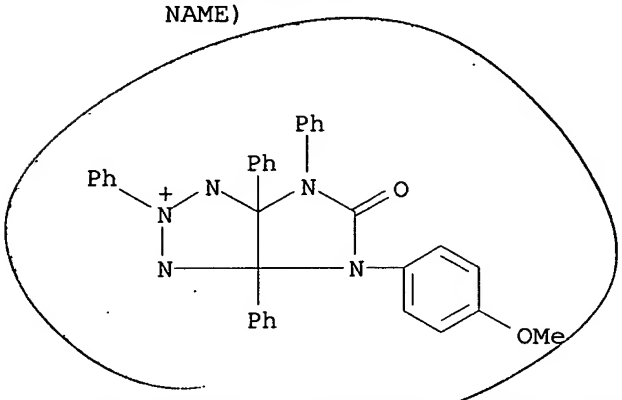
RN 144511-18-2 CAPLUS

CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-5-oxo-2,3a,4,6,6a-

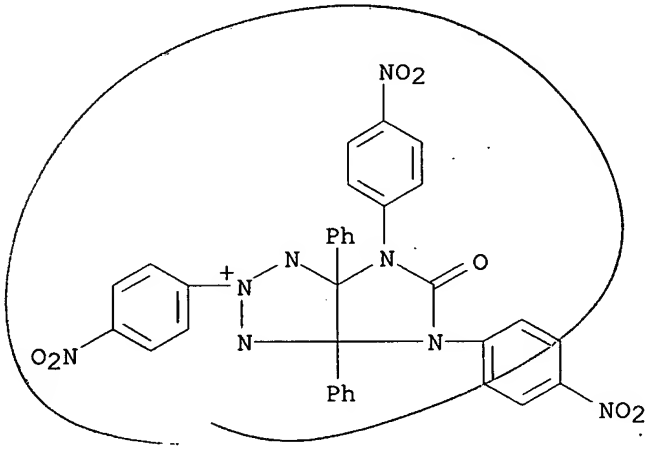
pentaphenyl-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-19-3 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-4-(4-methoxyphenyl)-5-oxo-2,3a,6,6a-tetraphenyl-, inner salt (9CI) (CA INDEX NAME)

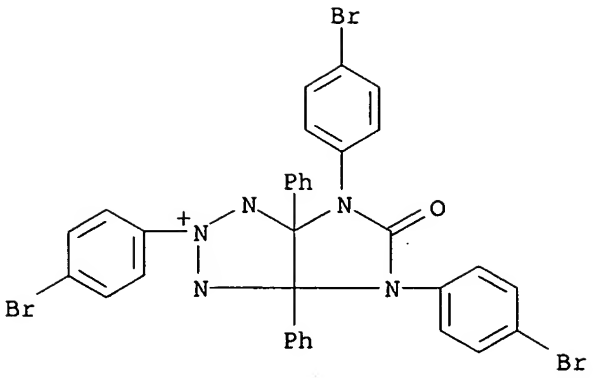


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-20-6 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-2,4,6-tris(4-nitrophenyl)-5-oxo-3a,6a-diphenyl-, inner salt (9CI) (CA INDEX NAME)

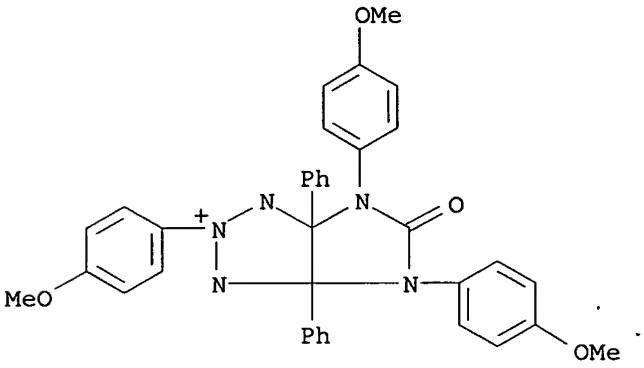


Tautomer

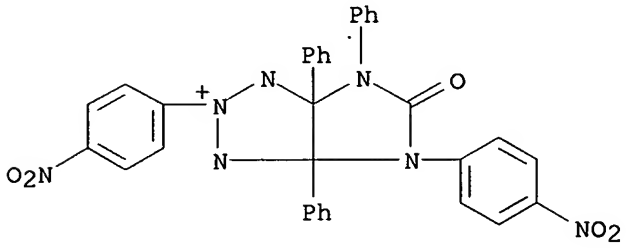
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-21-7 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 2,4,6-tris(4-bromophenyl)-1,3a,4,5,6,6a-hexahydro-5-oxo-3a,6a-diphenyl-, inner salt (9CI) (CA INDEX NAME)



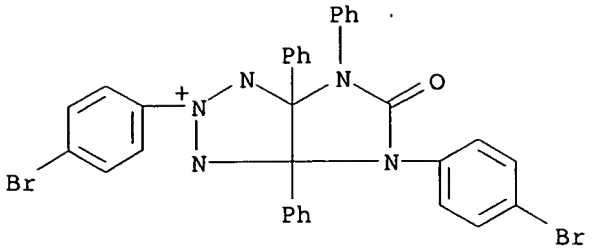
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-22-8 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-2,4,6-tris(4-methoxyphenyl)-5-oxo-3a,6a-diphenyl-, inner salt (9CI) (CA INDEX NAME)



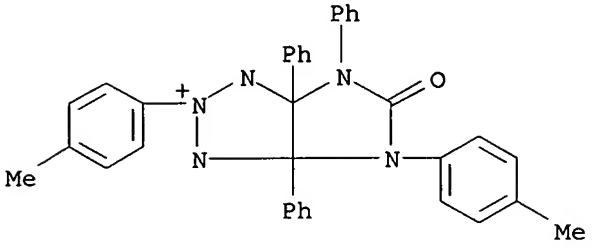
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-23-9 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-2,4-bis(4-nitrophenyl)-5-oxo-3a,6,6a-triphenyl-, inner salt (9CI) (CA INDEX NAME)



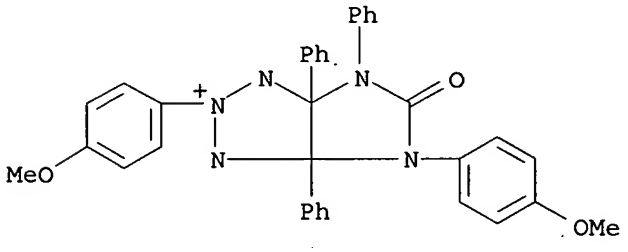
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-24-0 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 2,4-bis(4-bromophenyl)-1,3a,4,5,6,6a-hexahydro-5-oxo-3a,6,6a-triphenyl-, inner salt (9CI) (CA INDEX NAME)



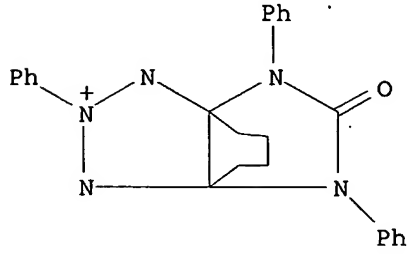
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-25-1 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-2,4-bis(4-methylphenyl)-5-oxo-3a,6,6a-triphenyl-, inner salt (9CI) (CA INDEX NAME)



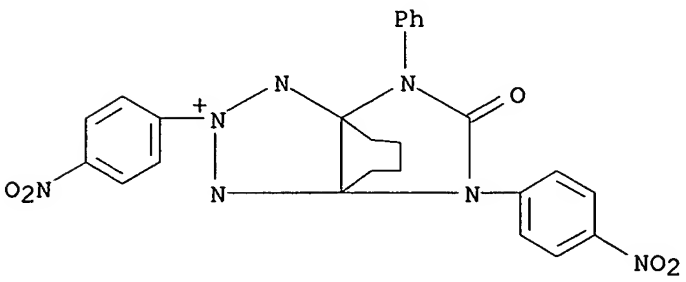
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-26-2 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-2,4-bis(4-methoxyphenyl)-5-oxo-3a,6,6a-triphenyl-, inner salt (9CI) (CA INDEX NAME)



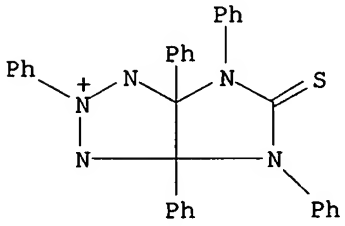
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-27-3 CAPLUS
CN 3a,7a-(Iminomethanimino)-1H-benzotriazolium, 4,5,6,7-tetrahydro-9-oxo-2,8,10-triphenyl-, inner salt (9CI) (CA INDEX NAME)



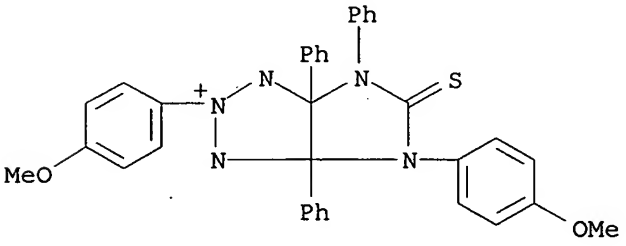
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-28-4 CAPLUS
CN 3a,7a-(Iminomethanimino)-1H-benzotriazolium, 4,5,6,7-tetrahydro-2,8-bis(4-nitrophenyl)-9-oxo-10-phenyl-, inner salt (9CI) (CA INDEX NAME)



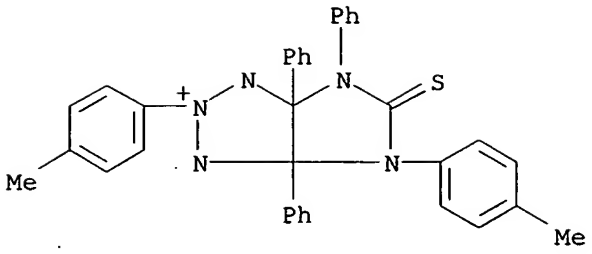
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-29-5 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-2,3a,4,6,6a-pentaphenyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



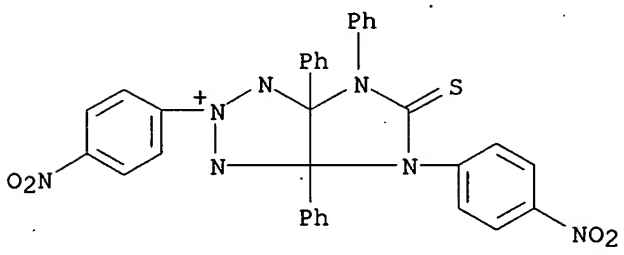
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-30-8 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-2,4-bis(4-methoxyphenyl)-3a,6,6a-triphenyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



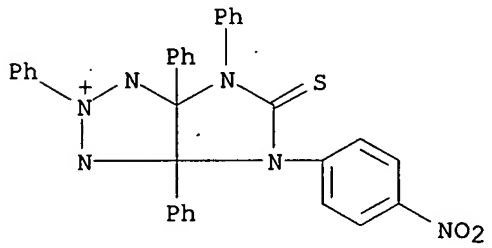
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-31-9 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-2,4-bis(4-methylphenyl)-3a,6,6a-triphenyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



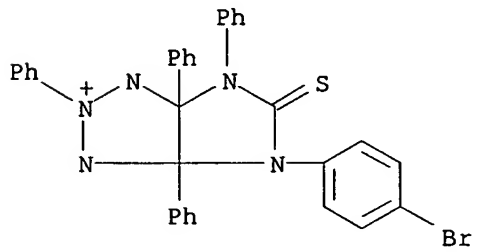
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-32-0 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-2,4-bis(4-nitrophenyl)-3a,6,6a-triphenyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



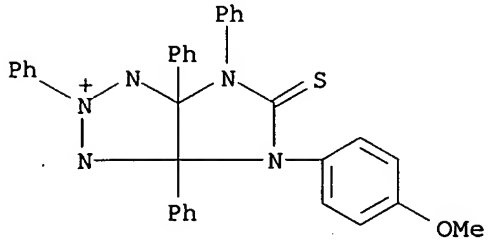
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-33-1 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-4-(4-nitrophenyl)-2,3a,6,6a-tetraphenyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



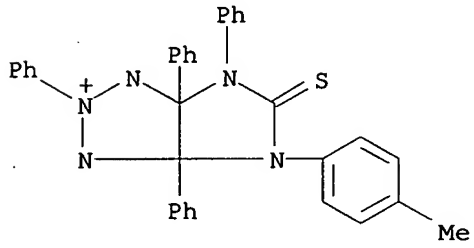
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-34-2 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 4-(4-bromophenyl)-1,3a,4,5,6,6a-hexahydro-2,3a,6,6a-tetraphenyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



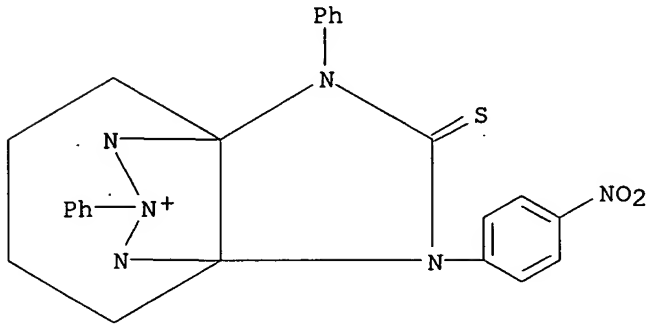
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-35-3 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-4-(4-methoxyphenyl)-2,3a,6,6a-tetraphenyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



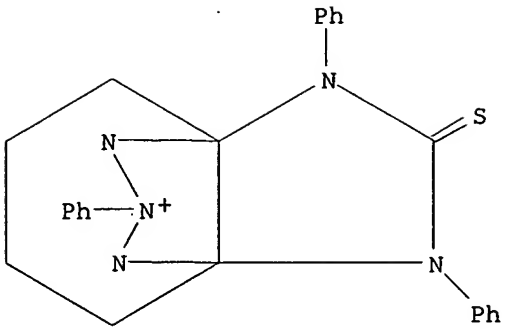
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-36-4 CAPLUS
CN Imidazo[4,5-d]-1,2,3-triazolium, 1,3a,4,5,6,6a-hexahydro-4-(4-methylphenyl)-2,3a,6,6a-tetraphenyl-5-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-37-5 CAPLUS
CN 3a,7a-(Iminomethanimino)-1H-benzotriazolium, 4,5,6,7-tetrahydro-8-(4-nitrophenyl)-2,10-diphenyl-9-thioxo-, inner salt (9CI) (CA INDEX NAME)

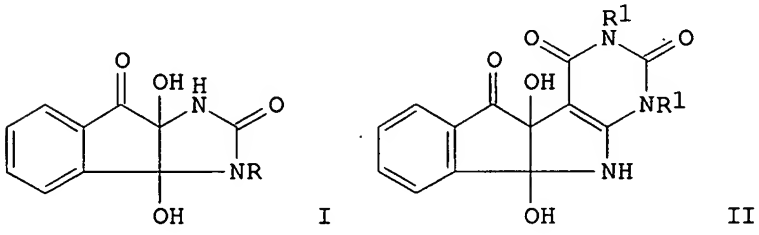


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 144511-38-6 CAPLUS
CN 3a,7a-(Iminomethanimino)-1H-benzotriazolium, 4,5,6,7-tetrahydro-2,8,10-triphenyl-9-thioxo-, inner salt (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L38 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1985:498575 CAPLUS
DOCUMENT NUMBER: 103:98575
TITLE: Anticonvulsive properties of newly-synthesized indenoimidazolediones
AUTHOR(S): Chatterjie, Nithiananda; Opoku-Ofori, Philip; Alexander, George J.
CORPORATE SOURCE: N. Y. State Inst. Basic Res. Dev. Disabil., Staten Island, NY, 10314, USA
SOURCE: Research Communications in Chemical Pathology and Pharmacology (1985), 47(2), 297-300
CODEN: RCOCB8; ISSN: 0034-5164
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:98575
GI

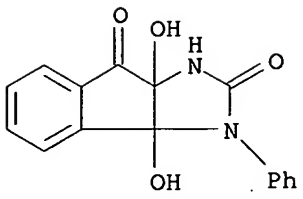


AB Compds. I; R = Ph **[29328-09-4]**, I; R = CH2CH:CH2 [97885-14-8], I; R = Bu [97885-15-9], II; R' = H [97885-16-0], and II; R' = Me [97885-17-1] were prepared by condensation of ninhydrin [485-47-2] with the appropriate monosubstituted ureas or 6-aminouracil derivs. All compds., except the Bu derivative, showed anticonvulsant activity in mice against seizures induced by Metrazole, but not against those induced by electroshock. At a dose of 100 mg/kg, which approximated the anticonvulsant ED50, spontaneous motor activity was decreased by Me-II, increased by H-I, and unaffected by the other compds. The CH2CH:CH2 derivative of I, which showed the highest anticonvulsant activity (ED50 = 68.76 mg/kg), showed no neurotoxicity up to 300 mg/kg but showed neurotoxicity at 590.2 mg/kg in 50% of the animals.

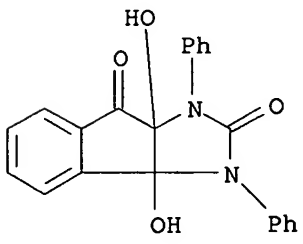
IT **29328-09-4**
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(anticonvulsant activity and toxicity of)

RN 29328-09-4 CAPLUS

CN Indeno[1,2-d]imidazole-2,8-dione, 1,3,3a,8a-tetrahydro-3a,8a-dihydroxy-3-phenyl- (8CI, 9CI) (CA INDEX NAME)



L38 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1976:17220 CAPLUS
DOCUMENT NUMBER: 84:17220
TITLE: Reaction of ninhydrin with urea and N-substituted ureas
AUTHOR(S): Crooks, Peter A.; Deeks, Trevor
CORPORATE SOURCE: Dep. Pharm., Univ. Manchester, Manchester, UK
SOURCE: Chemistry & Industry (London, United Kingdom) (1975), (18), 793-4
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The tautomeric 2-hydroxy-2-ureidoindane-1,3-dione structure proposed by M. Polonovski and F. Moreno-Martin (1935) for the reaction product of ninhydrin and urea is incorrect, the correct structure being I. Similar products are formed by reaction of (MeNH)2CO and (PhNH)2CO with ninhydrin 24-30 hr in refluxing C6H6. Reaction of Me2NCONH2 with ninhydrin 5 min at 80° in water gave 64% of the indanedione II.
IT **58137-72-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 58137-72-7 CAPLUS
CN Indeno[1,2-d]imidazole-2,8-dione, 1,3,3a,8a-tetrahydro-3a,8a-dihydroxy-1,3-diphenyl- (9CI) (CA INDEX NAME)

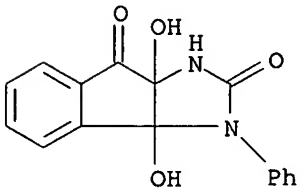


L38 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1974:449617 CAPLUS
DOCUMENT NUMBER: 81:49617
TITLE: Transformations of substituted tetrahydro-8H-indeno[1,2-d]imidazoles in concentrated sulfuric acid
AUTHOR(S): Arens, A.; Grunsbergs, F.; Jurgevica, I.
CORPORATE SOURCE: Rizh. Politekh. Inst., Riga, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1974), (4), 549-51
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.

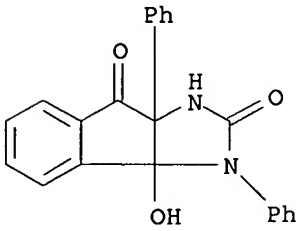
AB Spiroimidazolidinephthalans I (R1 = H, Me; R2 = H, Ph; R3 = OH, OMe) were obtained in 35-72% yield by treating the indenoimidazoles II with concentrated H2SO4 to give an intermediate which cyclodehydrated. Addnl. obtained were 49-61% imidaz-oles III (R1 = R2 = H, R3 = OH; R1 = PhCH2, R2 = R3 = Ph; R1 = H, R2 = R3 = Ph) which were cyclodehydrated to yield 34-80% imidazoloisoindolines IV (R1 = H, Me; R3 = OH, OMe).

IT **29328-09-4 29328-10-7 29328-12-9 53132-86-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sulfuric acid)

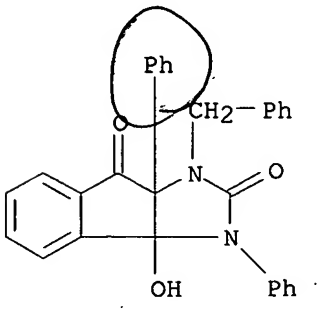
RN 29328-09-4 CAPLUS
CN Indeno[1,2-d]imidazole-2,8-dione, 1,3,3a,8a-tetrahydro-3a,8a-dihydroxy-3-phenyl- (8CI, 9CI) (CA INDEX NAME)



RN 29328-10-7 CAPLUS
CN Indeno[1,2-d]imidazole-2,8-dione, 1,3,3a,8a-tetrahydro-3a-hydroxy-3,8a-diphenyl- (8CI, 9CI) (CA INDEX NAME)

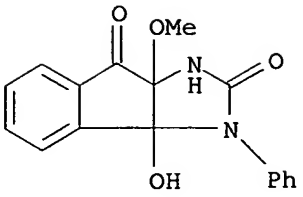


RN 29328-12-9 CAPLUS
CN Indeno[1,2-d]imidazole-2,8-dione, 1,3,3a,8a-tetrahydro-3a-hydroxy-3,8a-diphenyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

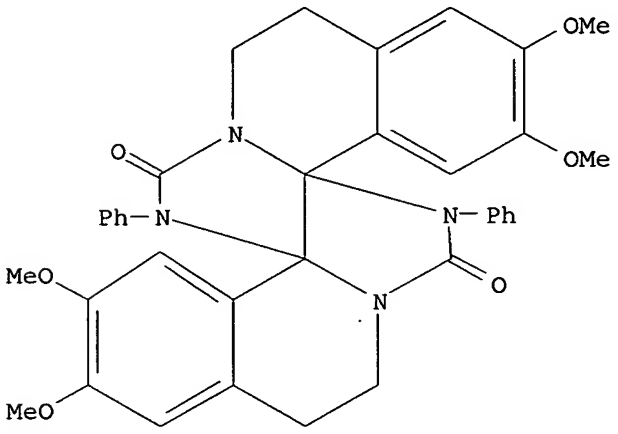


Yes, but no journal

RN 53132-86-8 CAPLUS
CN Indeno[1,2-d]imidazole-2,8-dione, 1,3,3a,8a-tetrahydro-3a-hydroxy-8a-methoxy-3-phenyl- (9CI) (CA INDEX NAME)

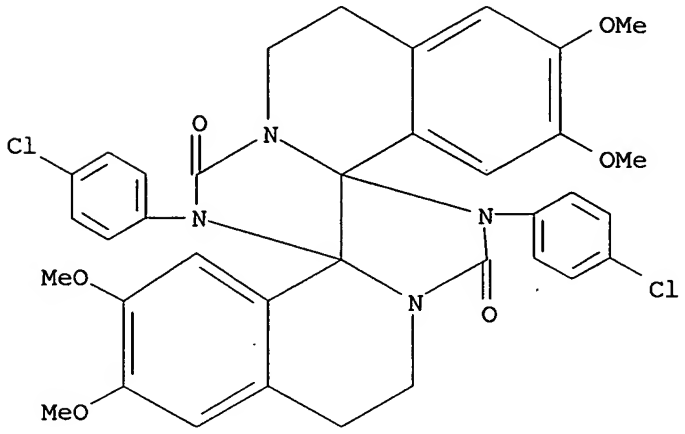


L38 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1973:97610 CAPLUS
DOCUMENT NUMBER: 78:97610
TITLE: Reaction of conjugated systems containing nitrogen. IV. Reaction of conjugated 1,2-diimines with isocyanates
AUTHOR(S): Sakamoto, Masanori; Tomimatsu, Yoshio; Miyazawa, Kyoko; Tokoro, Kazuhiko
CORPORATE SOURCE: Meiji Coll. Pharm., Tokyo, Japan
SOURCE: Yakugaku Zasshi (1972), 92(12), 1462-7
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI For diagram(s), see printed CA Issue.
AB Reaction of conjugated 1,2-diimines with isocyanates was investigated. 6,6',7,7'-Tetramethoxy-3,3',4,4'-tetrahydro-1,1'-biisoquinoline (I) reacted with RC6H4NCO, giving criss-cross type 1:2-adducts II (R = Ph, p-ClC6H4, PhCO (III), etc. Behavior of N,N'-bis(cyclohexyl)ethylenediimin e (IV) was different depending on reaction conditions. Reaction of IV with III, at room temperature afforded 1:2-adduct V through 1,2-cycloaddn., but in boiling xylene gave a criss-cross type 1:2-adduct VI (R = H). N,N'-bis(cyclohexyl)butylene-2,3-diimine reacted with III in boiling xylene to give VI (R = Me).
IT **40721-92-4P 40721-93-5P 40721-94-6P 40721-95-7P 40721-96-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40721-92-4 CAPLUS
CN Isoquino[2'',1'':3',4']imidazo[4',5':4,5]imidazo[5,1-a]isoquinoline-6,15(5H,14H)-dione, 8,9,17,18-tetrahydro-2,3,11,12-tetramethoxy-5,14-diphenyl- (9CI) (CA INDEX NAME)

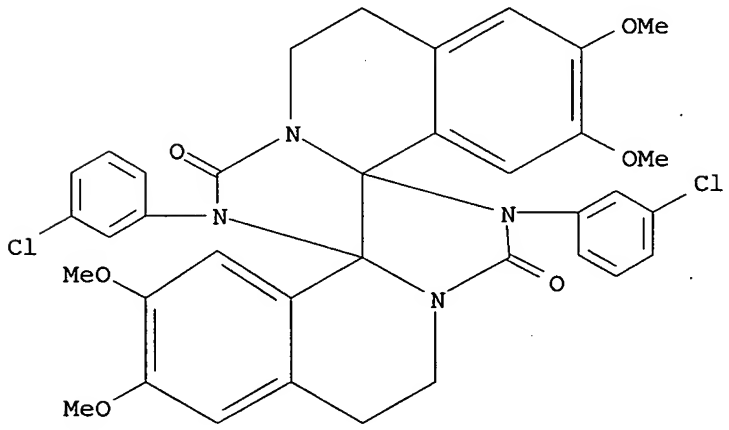


RN 40721-93-5 CAPLUS
CN Isoquino[2'',1'':3',4']imidazo[4',5':4,5]imidazo[5,1-a]isoquinoline-

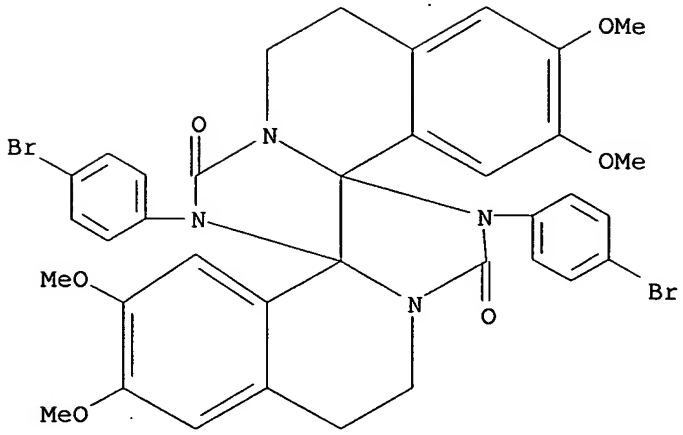
6,15(5H,14H)-dione, 5,14-bis(4-chlorophenyl)-8,9,17,18-tetrahydro-2,3,11,12-tetramethoxy- (9CI) (CA INDEX NAME)



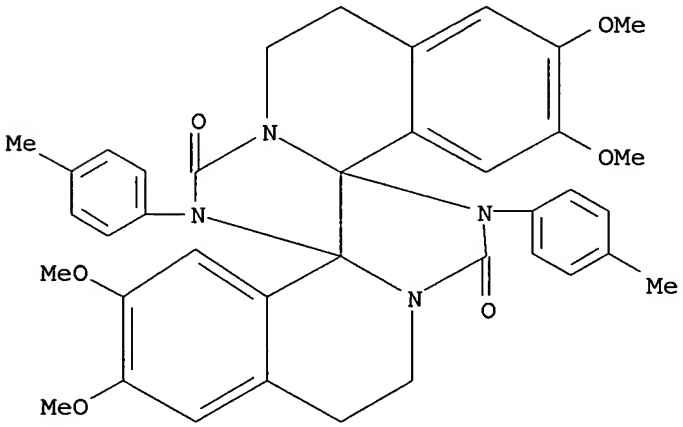
RN 40721-94-6 CAPLUS
CN Isoquino[2'',1'':3',4']imidazo[4',5':4,5]imidazo[5,1-a]isoquinoline-6,15(5H,14H)-dione, 5,14-bis(3-chlorophenyl)-8,9,17,18-tetrahydro-2,3,11,12-tetramethoxy- (9CI) (CA INDEX NAME)



RN 40721-95-7 CAPLUS
CN Isoquino[2'',1'':3',4']imidazo[4',5':4,5]imidazo[5,1-a]isoquinoline-6,15(5H,14H)-dione, 5,14-bis(4-bromophenyl)-8,9,17,18-tetrahydro-2,3,11,12-tetramethoxy- (9CI) (CA INDEX NAME)



RN 40721-96-8 CAPLUS
CN Isoquino[2'',1'':3',4']imidazo[4',5':4,5]imidazo[5,1-a]isoquinoline-6,15(5H,14H)-dione, 8,9,17,18-tetrahydro-2,3,11,12-tetramethoxy-5,14-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

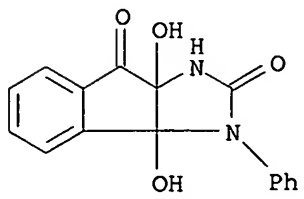


L38 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1970:508911 CAPLUS
DOCUMENT NUMBER: 73:108911
TITLE: Spectra and structure of 2-carbamido-1,3-indandiones
AUTHOR(S): Arens, Augusts; Jurgevica, I.; Grunsbergs, F.; Lencbergs, I.
CORPORATE SOURCE: Rizh. Politekh. Inst., Riga, USSR
SOURCE: Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija (1970), (3), 323-6
CODEN: LZAKAM; ISSN: 0002-3248
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB The uv and ir spectra of the title compds. were studied. The products of the interaction of ninhydrin with urea as well as N-methyl- and N-phenylurea have the indanonoimidazolone structure I rather than the ninhydrylurea structure II. The latter structure was confirmed only for the ninhydrin-N,N-dimethylurea interaction product.
IT **29328-09-4 29328-10-7 29328-11-8**
29328-12-9
RL: PRP (Properties)

(spectrum of, ir)

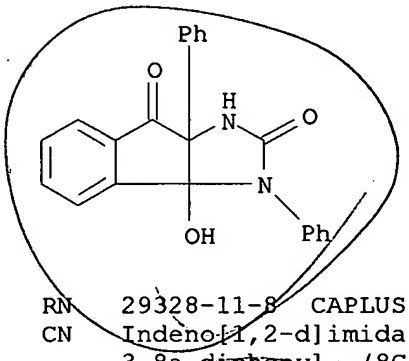
RN 29328-09-4 CAPLUS

CN Indeno[1,2-d]imidazole-2,8-dione, 1,3,3a,8a-tetrahydro-3a,8a-dihydroxy-3-phenyl- (8CI, 9CI) (CA INDEX NAME)



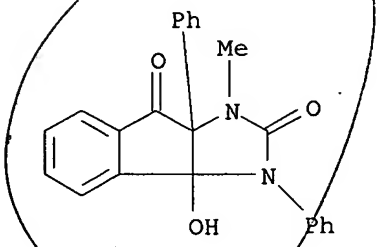
RN 29328-10-7 CAPLUS

CN Indeno[1,2-d]imidazole-2,8-dione, 1,3,3a,8a-tetrahydro-3a-hydroxy-3,8a-diphenyl- (8CI, 9CI) (CA INDEX NAME)



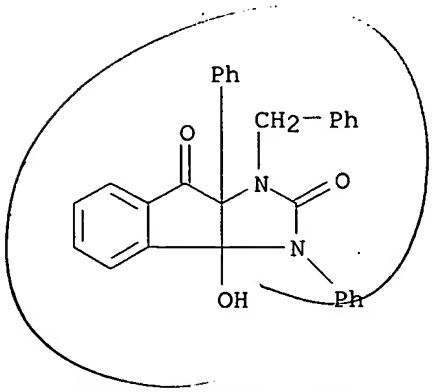
RN 29328-11-8 CAPLUS

CN Indeno[1,2-d]imidazole-2,8-dione, 1,3,3a,8a-tetrahydro-3a-hydroxy-1-methyl-3,8a-diphenyl- (8CI) (CA INDEX NAME)



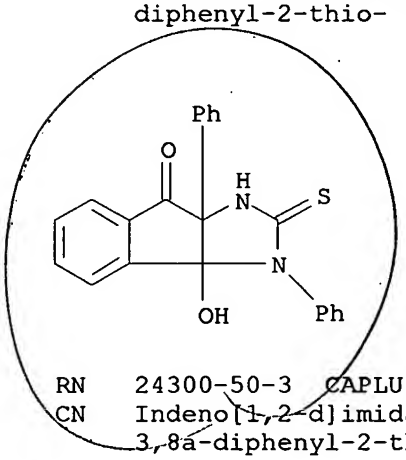
RN 29328-12-9 CAPLUS

CN Indeno[1,2-d]imidazole-2,8-dione, 1,3,3a,8a-tetrahydro-3a-hydroxy-3,8a-diphenyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

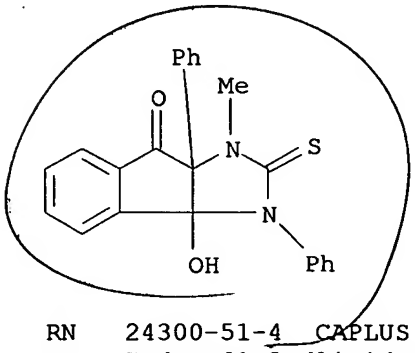


L38 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN

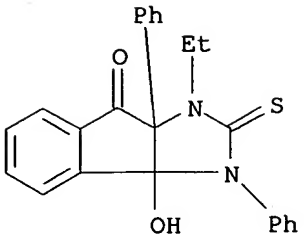
ACCESSION NUMBER: 1969:402804 CAPLUS
DOCUMENT NUMBER: 71:2804
TITLE: Substituted thiourea β-dicarbonyl compounds. IX. Spectroscopic study of 2-substituted N-[1,3-indandion-2-yl]thiourea and 2-(2-iminothiazolidin-3-yl]-2-substituted 1,3-indandiones
AUTHOR(S): Bite, Dz.; Valtere, S.; Arens, A.
CORPORATE SOURCE: Rizh. Politekh. Inst., Riga, USSR
SOURCE: Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija (1969), (1), 109-12
CODEN: LZAKAM; ISSN: 0002-3248
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Measurements of integral intensities of C:O bands showed that solid state I in dioxane solns. exists as form II. Detns. in the ir spectra were made for the following substances (R1 and R2 are given): H, Ph; Et, H; CH2Ph, H; Me, Ph; Et, Ph; CH2Ph, Ph. They react under the diketone form. Similarly the NH and CO groups of III cyclize to give IV.
IT **24300-47-8 24300-50-3 24300-51-4 24300-52-5**
RL: PRP (Properties)
(spectrum of, ir)
RN 24300-47-8 CAPLUS
CN Indeno[1,2-d]imidazole-2,8-dione, 1,3,3a,8a-tetrahydro-3a-hydroxy-3,8a-diphenyl-2-thio- (8CI) (CA INDEX NAME)



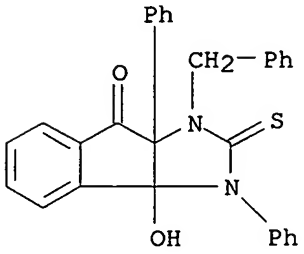
RN 24300-50-3 CAPLUS
CN Indeno[1,2-d]imidazole-2,8-dione, 1,3,3a,8a-tetrahydro-3a-hydroxy-1-methyl-3,8a-diphenyl-2-thio- (8CI) (CA INDEX NAME)



RN 24300-51-4 CAPLUS
CN Indeno[1,2-d]imidazole-2,8-dione, 1-ethyl-1,3,3a,8a-tetrahydro-3a-hydroxy-3,8a-diphenyl-2-thio- (8CI) (CA INDEX NAME)



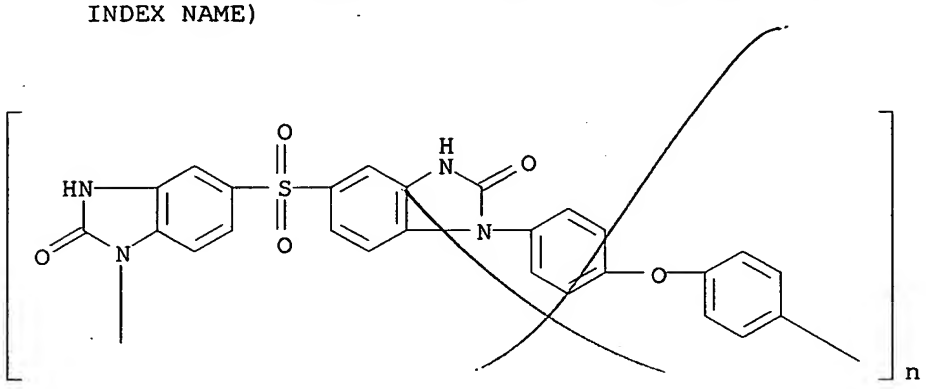
RN 24300-52-5 CAPLUS
CN Indeno[1,2-d]imidazole-2,8-dione, 1-benzyl-1,3,3a,8a-tetrahydro-3a-hydroxy-3,8a-diphenyl-2-thio- (8CI) (CA INDEX NAME)




```
=> d his

     (FILE 'HOME' ENTERED AT 09:17:06 ON 04 APR 2005)

     FILE 'REGISTRY' ENTERED AT 09:17:13 ON 04 APR 2005
L1             STRUCTURE UPLOADED
L2           1 S L1
L3          12 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 09:17:46 ON 04 APR 2005
L4           1 S L3
L5             STRUCTURE UPLOADED
               S L5

     FILE 'REGISTRY' ENTERED AT 09:21:23 ON 04 APR 2005
L6           0 S L5

     FILE 'CAPLUS' ENTERED AT 09:21:24 ON 04 APR 2005
L7           0 S L6

     FILE 'REGISTRY' ENTERED AT 09:21:29 ON 04 APR 2005
L8             STRUCTURE UPLOADED
L9          12 S L8 FULL

     FILE 'CAPLUS' ENTERED AT 09:22:04 ON 04 APR 2005
L10          1 S L9

     FILE 'BEILSTEIN' ENTERED AT 09:22:32 ON 04 APR 2005
L11          0 S L3
L12          0 S L8
L13          0 S L9

     FILE 'CAOLD' ENTERED AT 09:23:16 ON 04 APR 2005
L14          0 S L3
```

```
L15             0 S L9

     FILE 'CASREACT' ENTERED AT 09:23:41 ON 04 APR 2005
L16             0 S L3
L17             0 S L9

     FILE 'REGISTRY' ENTERED AT 09:26:56 ON 04 APR 2005
L18               STRUCTURE UPLOADED
L19             0 S L18
L20            12 S L18 FULL

     FILE 'CAPLUS' ENTERED AT 09:27:32 ON 04 APR 2005
L21             1 S L20

     FILE 'REGISTRY' ENTERED AT 09:30:47 ON 04 APR 2005
L22               STRUCTURE UPLOADED
L23            36 S L22
L24          1533 S L22 FULL

     FILE 'CAPLUS' ENTERED AT 09:31:20 ON 04 APR 2005
L25           438 S L24

     FILE 'REGISTRY' ENTERED AT 09:35:36 ON 04 APR 2005
L26               STRUCTURE UPLOADED
L27            34 S L26
L28          1438 S L26 FULL

     FILE 'CAPLUS' ENTERED AT 09:36:47 ON 04 APR 2005
L29           421 S L28
L30               STRUCTURE UPLOADED
                  S L30

     FILE 'REGISTRY' ENTERED AT 09:38:14 ON 04 APR 2005
L31             1 S L30

     FILE 'CAPLUS' ENTERED AT 09:38:14 ON 04 APR 2005
L32             1 S L31

     FILE 'REGISTRY' ENTERED AT 09:38:21 ON 04 APR 2005
L33               STRUCTURE UPLOADED
L34            39 S L33 FULL

     FILE 'CAPLUS' ENTERED AT 09:38:51 ON 04 APR 2005
L35             7 S L34

     FILE 'REGISTRY' ENTERED AT 09:42:43 ON 04 APR 2005
L36               STRUCTURE UPLOADED
L37            64 S L36 FULL

     FILE 'CAPLUS' ENTERED AT 09:43:19 ON 04 APR 2005
L38            14 S L37

=> d L25 ibib hitstr 350-399

L25  ANSWER 350 OF 438  CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         1977:160943  CAPLUS
DOCUMENT NUMBER:          86:160943
TITLE:                    Reverse osmosis membranes from aromatic polymers
AUTHOR(S):                Hara, S.; Mori, K.; Taketani, Y.; Seno, M.
CORPORATE SOURCE:         Cent. Res. Inst., Teijin Ltd., Tokyo, Japan
SOURCE:                   Proceedings of the International Symposium on Fresh
                          Water from the Sea (1976), 4, 53-62
                          CODEN: PSFSDZ; ISSN: 0378-2298
```

DOCUMENT TYPE: Journal
LANGUAGE: English
IT **62628-01-7**
RL: OCCU (Occurrence)
(reverse osmosis membrane, permeability of)
RN 62628-01-7 CAPLUS
CN Poly[(2,3-dihydro-2-oxo-1H-benzimidazole-1,5-diyl)sulfonyl(2,3-dihydro-2-oxo-1H-benzimidazole-5,1-diyl)-1,4-phenyleneoxy-1,4-phenylene] (9CI) (CA INDEX NAME)

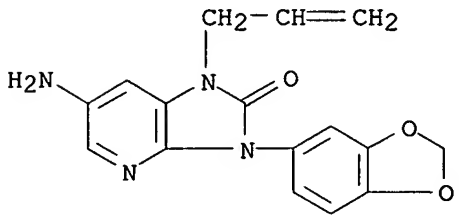


L25 ANSWER 351 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:106592 CAPLUS
DOCUMENT NUMBER: 86:106592
TITLE: 1,3-Dihydroimidazo[4,5-b]pyridin-2-ones and thiones
INVENTOR(S): Clark, Robert Long; Pessolano, Arsenio A.; Shen, Tsung-Ying
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Ger. Offen., 83 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

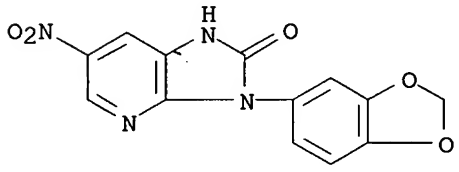
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2623469	A1	19761216	DE 1976-2623469	19760525
DK 7602100	A	19761129	DK 1976-2100	19760512
SE 422799	B	19820329	SE 1976-5399	19760512
SE 422799	C	19820708		
NL 7605131	A	19761130	NL 1976-5131	19760513
AU 7614055	A1	19771124	AU 1976-14055	19760518
AU 510273	B2	19800619		
FR 2312248	A1	19761224	FR 1976-15430	19760521
FR 2312248	B1	19790921		
BE 842255	A1	19761126	BE 1976-167360	19760526
ZA 7603164	A	19770525	ZA 1976-3164	19760526
ES 448280	A1	19780301	ES 1976-448280	19760526
GB 1542940	A	19790328	GB 1976-21886	19760526
HU 20154	O	19810627	HU 1976-ME1980	19760527
HU 177865	P	19820128		
JP 51143696	A2	19761210	JP 1976-61324	19760528
CH 635586	A	19830415	CH 1976-6718	19760528
PRIORITY APPLN. INFO.:			US 1975-601672 A	19750528

IT **61964-24-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of)
RN 61964-24-7 CAPLUS

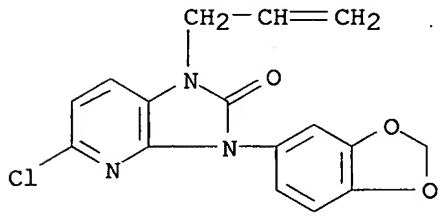
CN 2H-Imidazo[4,5-b]pyridin-2-one, 6-amino-3-(1,3-benzodioxol-5-yl)-1,3-dihydro-1-(2-propenyl)- (9CI) (CA INDEX NAME)



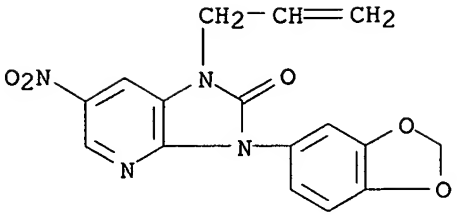
IT **61964-14-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and alkylation of)
RN 61964-14-5 CAPLUS
CN 2H-Imidazo[4,5-b]pyridin-2-one, 3-(1,3-benzodioxol-5-yl)-1,3-dihydro-6-nitro- (9CI) (CA INDEX NAME)



IT **61964-23-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amination of)
RN 61964-23-6 CAPLUS
CN 2H-Imidazo[4,5-b]pyridin-2-one, 3-(1,3-benzodioxol-5-yl)-5-chloro-1,3-dihydro-1-(2-propenyl)- (9CI) (CA INDEX NAME)



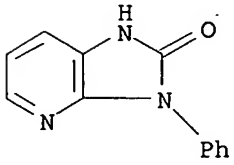
IT **61964-15-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)
RN 61964-15-6 CAPLUS
CN 2H-Imidazo[4,5-b]pyridin-2-one, 3-(1,3-benzodioxol-5-yl)-1,3-dihydro-6-nitro-1-(2-propenyl)- (9CI) (CA INDEX NAME)



IT **41010-50-8P 41010-72-4P 41010-73-5P**
41010-74-6P 41010-75-7P 41082-24-0P
61962-84-3P 61962-85-4P 61962-86-5P
61962-87-6P 61962-88-7P 61962-89-8P
61962-90-1P 61962-91-2P 61962-92-3P
61962-94-5P 61962-95-6P 61962-96-7P
61962-97-8P 61962-98-9P 61962-99-0P
61963-00-6P 61963-01-7P 61963-02-8P
61963-03-9P 61963-04-0P 61963-06-2P
61963-07-3P 61963-08-4P 61963-09-5P
61963-10-8P 61963-11-9P 61963-12-0P
61963-13-1P 61963-14-2P 61963-15-3P
61963-17-5P 61963-18-6P 61963-19-7P
61963-20-0P 61963-21-1P 61963-22-2P
61963-23-3P 61963-24-4P 61963-25-5P
61963-26-6P 61963-27-7P 61963-28-8P
61963-29-9P 61963-30-2P 61963-31-3P
61963-32-4P 61963-33-5P 61963-34-6P
61963-35-7P 61963-36-8P 61963-37-9P
61963-38-0P 61963-39-1P 61963-40-4P
61963-41-5P 61963-42-6P 61963-43-7P
61963-44-8P 61963-45-9P 61963-46-0P
61963-47-1P 61963-48-2P 61963-49-3P
61963-50-6P 61963-51-7P 61963-52-8P
61963-54-0P 61963-55-1P 61963-56-2P
61963-57-3P 61963-58-4P 61963-59-5P
61963-60-8P 61964-09-8P 61964-10-1P
61964-11-2P 61964-16-7P 61964-17-8P
61964-18-9P 61964-19-0P 61964-22-5P
61964-25-8P 61964-26-9P 61964-29-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

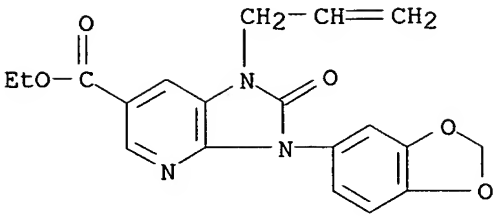
RN 41010-50-8 CAPLUS

CN 2H-Imidazo[4,5-b]pyridin-2-one, 1,3-dihydro-3-phenyl- (9CI) (CA INDEX NAME)

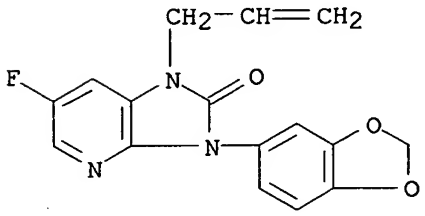


RN 41010-72-4 CAPLUS

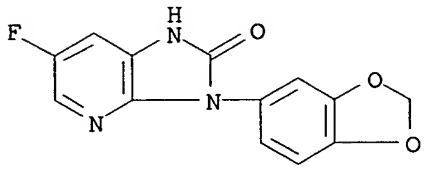
CN 2H-Imidazo[4,5-b]pyridin-2-one, 1,3-dihydro-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



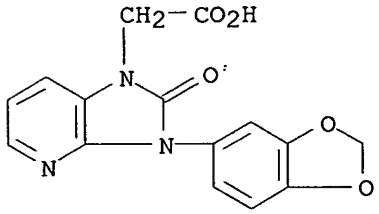
RN 61964-26-9 CAPLUS
CN 2H-Imidazo[4,5-b]pyridin-2-one, 3-(1,3-benzodioxol-5-yl)-6-fluoro-1,3-dihydro-1-(2-propenyl)- (9CI) (CA INDEX NAME)



RN 61964-29-2 CAPLUS
CN 2H-Imidazo[4,5-b]pyridin-2-one, 3-(1,3-benzodioxol-5-yl)-6-fluoro-1,3-dihydro- (9CI) (CA INDEX NAME)

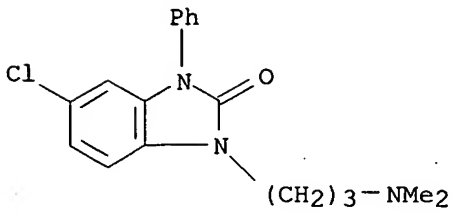


IT **61963-49-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thionyl chloride and morpholine)
RN 61963-49-3 CAPLUS
CN 1H-Imidazo[4,5-b]pyridine-1-acetic acid, 3-(1,3-benzodioxol-5-yl)-2,3-dihydro-2-oxo- (9CI) (CA INDEX NAME)



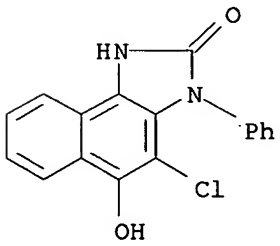
L25 ANSWER 352 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:72694 CAPLUS
DOCUMENT NUMBER: 86:72694
TITLE: Fused ring benzimidazole derivatives
INVENTOR(S): White, Alan Chapman; Black, Robin Michael

phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

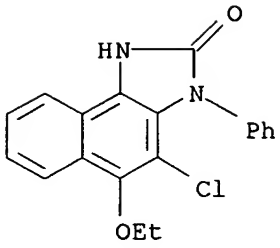


● HCl

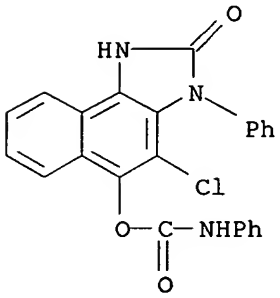
L25 ANSWER 381 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1970:530934 CAPLUS
DOCUMENT NUMBER: 73:130934
TITLE: Heterocyclizations. VIII. Unusual formation of 3-phenylnaphth[1,2-d]imidazole-2,5-diones
AUTHOR(S): Capuano, Lilly; Ebner, Wolfgang
CORPORATE SOURCE: Inst. Org. Chem., Univ. Saarland, Saarbruecken, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1970), 103(10), 3104-13
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 73:130934
IT **29540-88-3P 29540-89-4P 29540-90-7P**
29540-91-8P 29540-92-9P 29540-94-1P
29540-95-2P 29540-97-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 29540-88-3 CAPLUS
CN 2H-Naphth[1,2-d]imidazol-2-one, 4-chloro-1,3-dihydro-5-hydroxy-3-phenyl- (8CI) (CA INDEX NAME)



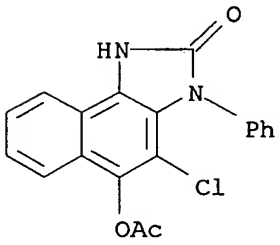
RN 29540-89-4 CAPLUS
CN 2H-Naphth[1,2-d]imidazol-2-one, 4-chloro-5-ethoxy-1,3-dihydro-3-phenyl- (8CI) (CA INDEX NAME)



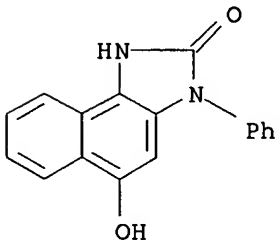
RN 29540-90-7 CAPLUS
CN 2H-Naphth[1,2-d]imidazol-2-one, 4-chloro-1,3-dihydro-5-hydroxy-3-phenyl-, carbanilate (ester) (8CI) (CA INDEX NAME)



RN 29540-91-8 CAPLUS
CN 2H-Naphth[1,2-d]imidazol-2-one, 4-chloro-1,3-dihydro-5-hydroxy-3-phenyl-, acetate (ester) (8CI) (CA INDEX NAME)

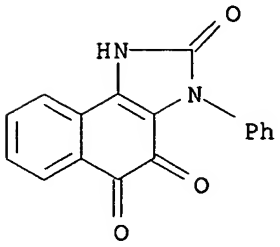


RN 29540-92-9 CAPLUS
CN 2H-Naphth[1,2-d]imidazol-2-one, 1,3-dihydro-5-hydroxy-3-phenyl- (8CI) (CA INDEX NAME)

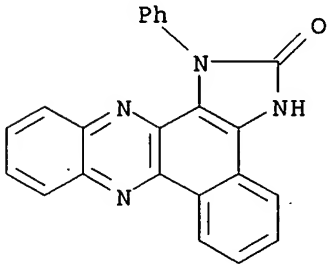


RN 29540-94-1 CAPLUS

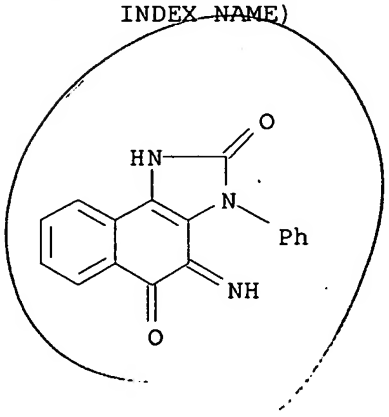
CN 2H-Naphth[1,2-d]imidazole-2,4,5-trione, 1,3-dihydro-3-phenyl- (8CI) (CA INDEX NAME)



RN 29540-95-2 CAPLUS
CN 2H-Benz[a]imidazo[4,5-c]phenazin-2-one, 1,3-dihydro-1-phenyl- (8CI) (CA INDEX NAME)



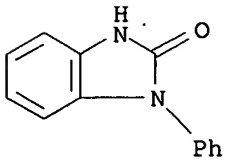
RN 29540-97-4 CAPLUS
CN 1H-Naphth[1,2-d]imidazole-2,5(3H,4H)-dione, 4-imino-3-phenyl- (8CI) (CA INDEX NAME)



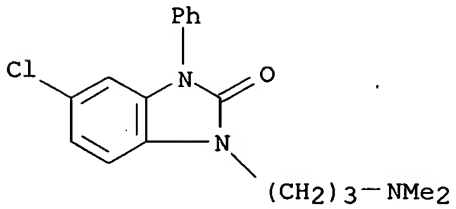
L25 ANSWER 382 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:	1970:477143 CAPLUS
DOCUMENT NUMBER:	73:77143
TITLE:	Syntheses of heterocyclic compounds. CCCLXV. Syntheses of azole derivatives. I. Formation of 1-substituted -3-hydroxy-1H-indazole and 1-substituted benzimidazolin-2-one derivatives by thermal reaction of N-substituted-N-arylcarbamoyl azides
AUTHOR(S):	Kametani, Tetsuji; Sota, Kaoru; Shio, Masahisa
CORPORATE SOURCE:	Pharm. Inst., Tohoku Univ., Sendai, Japan
SOURCE:	Journal of Heterocyclic Chemistry (1970), 7(4), 807-13 CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 73:77143

A. K.
CORPORATE SOURCE: Cairo Univ., Cairo, Egypt
SOURCE: Kogyo Kayaku Kyokaishi (1968), 29(2), 108-15
CODEN: KKKYAW; ISSN: 0368-5977
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **14813-85-5**
RL: USES (Uses)
(stabilizers, for explosives)
RN 14813-85-5 CAPLUS
CN 2H-Benzimidazol-2-one, 1,3-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



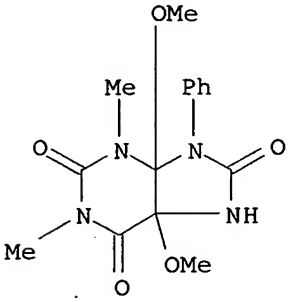
L25 ANSWER 392 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1969:95261 CAPLUS
DOCUMENT NUMBER: 70:95261
TITLE: Antidepressant of the 2-benzimidazolinone group
AUTHOR(S): Stille, Guenther; Lauener, Hans; Eichenberger, Erwin
CORPORATE SOURCE: Forschungsinst., Bern, Switz.
SOURCE: International Pharmacopsychiatry (1968), 1(3), 214-20
CODEN: INPHB6; ISSN: 0020-8272
DOCUMENT TYPE: Journal
LANGUAGE: German
IT **4913-61-5**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacology of)
RN 4913-61-5 CAPLUS
CN 2H-Benzimidazol-2-one, 5-chloro-1-[3-(dimethylamino)propyl]-1,3-dihydro-3-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



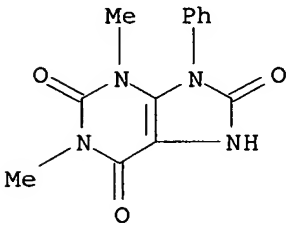
● HCl

L25 ANSWER 393 OF 438 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1969:77916 CAPLUS
DOCUMENT NUMBER: 70:77916
TITLE: Photoinduced reactions. XXIV. Photosensitized oxygenation of hydroxylated 9-phenylpurines
AUTHOR(S): Matsuura, Teruo; Saito, Isao
CORPORATE SOURCE: Kyoto Univ., Kyoto, Japan
SOURCE: Tetrahedron (1969), 25(3), 541-7
CODEN: TETRAB; ISSN: 0040-4020

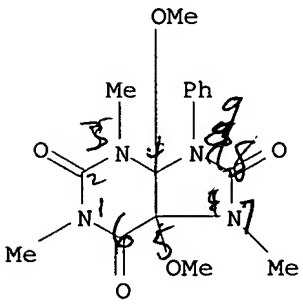
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 70:77916
IT **22305-91-5P 22305-92-6P 22305-93-7P 22305-94-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 22305-91-5 CAPLUS
CN Uric acid, dihydro-4,5-dimethoxy-1,3-dimethyl-9-phenyl- (8CI) (CA INDEX NAME)



RN 22305-92-6 CAPLUS
CN Uric acid, 1,3-dimethyl-9-phenyl- (8CI) (CA INDEX NAME)



RN 22305-93-7 CAPLUS
CN Uric acid, dihydro-4,5-dimethoxy-1,3,7-trimethyl-9-phenyl- (8CI) (CA INDEX NAME)



RN 22305-94-8 CAPLUS
CN Uric acid, dihydro-4,5-dimethoxy-9-phenyl- (8CI) (CA INDEX NAME)

10/681,924 4/4/05

FILE 'CAPLUS' ENTERED AT 15:32:45 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

text search
benzimidazol?
hexahydro!
and 2-oxo or 2-one

FILE COVERS 1907 - 4 Apr 2005 VOL 142 ISS 15
FILE LAST UPDATED: 3 Apr 2005 (20050403/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s benzimidazol?
L1        30723 BENZIMIDAZOL?

=> s 2(2w)oxo or 2(2w)one
        8338667 2
         143515 OXO
             21 OXOS
         143517 OXO
                (OXO OR OXOS)
          37435 2(2W)OXO
        8338667 2
        1945366 ONE
         156993 ONES
        2070693 ONE
                (ONE OR ONES)
         100413 2(2W)ONE
L2      133733 2(2W)OXO OR 2(2W)ONE

=> s L1 and hexahydro and L2
          27385 HEXAHYDRO
              1 HEXAHYDROS
          27386 HEXAHYDRO
                (HEXAHYDRO OR HEXAHYDROS)
L3          102 L1 AND HEXAHYDRO AND L2

=> d ibib 90-102

L3   ANSWER 90 OF 102  CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         1954:7161  CAPLUS
DOCUMENT NUMBER:          48:7161
ORIGINAL REFERENCE NO.:   48:1318a-i,1319a-i,1320a-i
TITLE:                    The nature of light-induced degradation products of
                          diazo derivatives. IV. The light reaction of
                          o-quinonediazides: photosyntheses of
                          cyclopentadiene derivatives
AUTHOR(S):                Sus, Oskar; Hoffmann, Hinrich; Rosenberger, Siegfried;
                          Kostka, Rudolf
CORPORATE SOURCE:         Kalle & Co., Wiesbaden-Biebrich, Germany
SOURCE:                   Ann. (1953), 579, 133-58
DOCUMENT TYPE:            Journal
```

LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 48:7161

L3 ANSWER 91 OF 102 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1952:10829 CAPLUS
DOCUMENT NUMBER: 46:10829
ORIGINAL REFERENCE NO.: 46:1898e-i,1899a-i,1900a-i
TITLE: Color and constitution. X. Absorption of the merocyanines
AUTHOR(S): Brooker, L. G. S.; Keyes, G. H.; Sprague, R. H.; VanDyke, R. H.; VanLare, E.; VanZandt, G.; White, F. L.; Cressman, H. W. J.; Dent, S. G., Jr.
CORPORATE SOURCE: Kodak Research Labs., Rochester, NY
SOURCE: Journal of the American Chemical Society (1951), 73, 5332-50
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

L3 ANSWER 92 OF 102 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1952:8890 CAPLUS
DOCUMENT NUMBER: 46:8890
ORIGINAL REFERENCE NO.: 46:1617g-i
TITLE: The effects of biologically active agents on fungi at different stages of growth
AUTHOR(S): Perlman, D.
CORPORATE SOURCE: 35 Edgehill St., Princeton, NJ
SOURCE: American Journal of Botany (1951), 38, 652-8
CODEN: AJBOAA; ISSN: 0002-9122
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

L3 ANSWER 93 OF 102 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1951:53187 CAPLUS
DOCUMENT NUMBER: 45:53187
ORIGINAL REFERENCE NO.: 45:9113c-d
TITLE: Nonspecificity of biotin activity for Leuconostoc
AUTHOR(S): Whiteside-Carlson, Virginia; Starnes, Willard R.; Rosano, Carmen L.; Carlson, Warner W.
CORPORATE SOURCE: Med. Coll. of Alabama, Birmingham
SOURCE: Proceedings of the Society for Experimental Biology and Medicine (1951), 77, 344-8
CODEN: PSEBAA; ISSN: 0037-9727
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

L3 ANSWER 94 OF 102 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1951:3754 CAPLUS
DOCUMENT NUMBER: 45:3754
ORIGINAL REFERENCE NO.: 45:666h-i
TITLE: Furoimidazoles
INVENTOR(S): Hofmann, Klaus
PATENT ASSIGNEE(S): Ciba Pharmaceutical Products, Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2520404		19500829	US	

L3 ANSWER 95 OF 102 CAPLUS COPYRIGHT 2005 ACS on STN

ε-caprolactam)
IT 2506-05-0, 1-**Benzimidazolecarboxanilide**, N-methyl-
(catalysts from Na caprolactam and, polymerization of ε-caprolactam)
IT 788-43-2, 2H-Azepin-**2-one**, 1-(2,2,3,3,4,4-hexafluoro-1-hydroxycyclobutyl)**hexahydro**-
(metal derivs., catalysts from urea derivs. and, in polymerization of lactams)
IT 788-43-2, 2H-Azepin-**2-one**, 1-(2,2,3,3,4,4-hexafluoro-1-hydroxycyclobutyl)**hexahydro**-
(polymerization of, 1-**benzimidazole** carboxanilide and Na salt of caprolactam as catalyst in)

=> d his

(FILE 'HOME' ENTERED AT 15:32:37 ON 04 APR 2005)

FILE 'CAPLUS' ENTERED AT 15:32:45 ON 04 APR 2005
L1 30723 S BENZIMIDAZOL?
L2 133733 S 2(2W)OXO OR 2(2W)ONE
L3 102 S L1 AND HEXAHYDRO AND L2

FILE 'CAPLUS' ENTERED AT 15:38:04 ON 04 APR 2005

=> fil caold
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	148.75	203.31

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-23.36	-26.28

FILE 'CAOLD' ENTERED AT 15:40:06 ON 04 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s L3
795 BENZIMIDAZOL?
269 HEXAHYDRO
77098 2
3062 OXO
382 2(2W)OXO
77098 2
5615 ONE
841 ONES
6436 ONE

(ONE OR ONES)
791 2(2W)ONE
L4 0 L1 AND HEXAHYDRO AND L2

=> fil beilstein
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	11.23	214.54

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-26.28

FILE 'BEILSTEIN' ENTERED AT 15:40:17 ON 04 APR 2005

FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON February 14, 2005

FILE COVERS 1771 TO 2004.
*** FILE CONTAINS 9,133,317 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in
separate documents and can not be searched together in one query.
Reaction data for BEILSTEIN compounds may be displayed
immediately with the display codes PRE (preparations) and REA
(reactions). A substance answer set retrieved after the search
for a chemical name, a compounds with available reaction
information by combining with PRE/FA, REA/FA or more generally
with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
between a BEILSTEIN compound and belonging reactions. For mo
detailed reaction searches BRNs can be searched as reaction
partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

****
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *
****

NEW
*** PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.**
*** NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.**

=> s L3
15182 BENZIMIDAZOL?
199980 HEXAHYDRO
6416083 2
797577 OXO
1 OXOS
797577 OXO
(OXO OR OXOS)
333493 2(2W)OXO
6416083 2
923977 ONE
77 ONES

```
        924004 ONE
                  (ONE OR ONES)
        341784 2(2W)ONE
L5          15 L1 AND HEXAHYDRO AND L2

=> d L5 1-15 ibib
'IBIB' IS NOT A VALID FORMAT FOR FILE 'BEILSTEIN'

The following are valid formats:

QRD --------- Query Related Data (IDE plus HIT)
IDE --------- Identification of Substance, plus Structure
ALL --------- All Display fields (Lengthy displaye)
CHE --------- Chemical Data
PHY --------- Physical Data
HIT --------- All fields containing hit terms
Hit terms will be highlighted in all IDE fields in the BEILSTEIN file
A maximum of 20 values are displayed in each single property field.
Use DISPLAY F<prop> for FULL format, e.g. FBP instead of BP.
For more information about display formats, and how to display
individual selected properties, enter 'HELP FORMAT' at an arrow
prompt, e.g. => HELP FORMAT.
ENTER DISPLAY FORMAT (QRD):hit

L5   ANSWER 1 OF 15 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

     Chemical Name (CN):          1-anilino-6-(tert-butyl)-1,3,4,5,6,7-
                                  hexahydro-2H-benzimidazol-2-one
     Autonom Name (AUN):          6-tert-butyl-1-phenylamino-
                                  1,3,4,5,6,7-hexahydro-benzoimidazol-2-
                                  one
     Autonom Name (AUN):          6-tert-butyl-1-phenylamino-
                                  1,3,4,5,6,7-hexahydro-benzoimidazol-2-
                                  one

L5   ANSWER 2 OF 15 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

     Chemical Name (CN):          1-anilino-1,3,4,5,6,7-hexahydro-2H-
                                  benzimidazol-2-one
     Autonom Name (AUN):          1-phenylamino-1,3,4,5,6,7-hexahydro-
                                  benzoimidazol-2-one
     Autonom Name (AUN):          1-phenylamino-1,3,4,5,6,7-hexahydro-
                                  benzoimidazol-2-one

L5   ANSWER 3 OF 15 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

     Chemical Name (CN):          2,3,4,5,6,7-Hexahydro-2-oxo-1H-
                                  benzimidazol-3-carbonsaeureamid
     Autonom Name (AUN):          2-oxo-2,3,4,5,6,7-hexahydro-
                                  benzoimidazole-1-carboxylic acid amide
     Autonom Name (AUN):          2-oxo-2,3,4,5,6,7-hexahydro-
                                  benzoimidazole-1-carboxylic acid amide

L5   ANSWER 4 OF 15 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

     Chemical Name (CN):          (3aα,4α,7α,7a.alpha
                                  .)-1,3,3a,4,7,7a-hexahydro-4,7-methano-2H-
                                  benzimidazol-2-one
     Autonom Name (AUN):          1,3,3a,4,7,7a-hexahydro-4,7-methano-
```

Autonom Name (AUN): **benzoimidazol-2-one**
1,3,3a,4,7,7a-hexahydro-4,7-methano-benzoimidazol-2-one

L5 ANSWER 5 OF 15 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Chemical Name (CN): **1-(2-ethoxyethyl)-2-(hexahydro-5-oxo-1H-1,4-diazepin-1-yl)-1H-benzimidazole**
Autonom Name (AUN): 1-<1-(2-ethoxy-ethyl)-1H-benzoimidazol-2-yl>-<1,4>diazepan-5-one

L5 ANSWER 6 OF 15 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Chemical Name (CN): **1-(2-ethoxyethyl)-2-(hexahydro-5-oxo-1H-1,4-diazepin-1-yl)-6-phenylmethoxy-1H-benzimidazole**
Autonom Name (AUN): 1-<6-benzyloxy-1-(2-ethoxy-ethyl)-1H-benzoimidazol-2-yl>-<1,4>diazepan-5-one

L5 ANSWER 7 OF 15 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Chemical Name (CN): **1-(2-ethoxyethyl)-2-(hexahydro-5-oxo-1H-1,4-diazepin-1-yl)-5-phenylmethoxy-1H-benzimidazole**
Autonom Name (AUN): 1-<5-benzyloxy-1-(2-ethoxy-ethyl)-1H-benzoimidazol-2-yl>-<1,4>diazepan-5-one

L5 ANSWER 8 OF 15 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Chemical Name (CN): **(3aα,4α,7α,7a.alpha.)-1,3-diacetyl-1,3,3a,4,7,7a-hexahydro-4,7-methano-2H-benzimidazol-2-one**
Autonom Name (AUN): **1,3-diacetyl-1,3,3a,4,7,7a-hexahydro-4,7-methano-benzoimidazol-2-one**
Autonom Name (AUN): **1,3-diacetyl-1,3,3a,4,7,7a-hexahydro-4,7-methano-benzoimidazol-2-one**

L5 ANSWER 9 OF 15 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Chemical Name (CN): **(4R)-4,8,8-trimethyl-(3aξ,7aξ)-hexahydro-4,7-methano-benzimidazol-2-one; hydrochloride**

L5 ANSWER 10 OF 15 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

Chemical Name (CN): **2,3,3a,4,7,7a-hexahydro-1H-benzimidazol-2-one**
Autonom Name (AUN): **1,3,3a,4,7,7a-hexahydro-benzoimidazol-2-one**
Autonom Name (AUN): **1,3,3a,4,7,7a-hexahydro-benzoimidazol-2-one**

L5 ANSWER 11 OF 15 BEILSTEIN COPYRIGHT 2005 BEILSTEIN MDL on STN

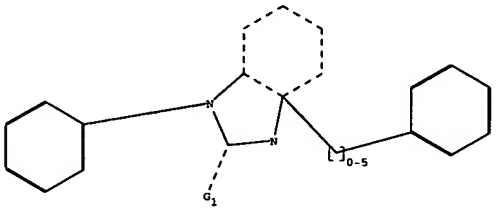
Chemical Derivative:
CDER

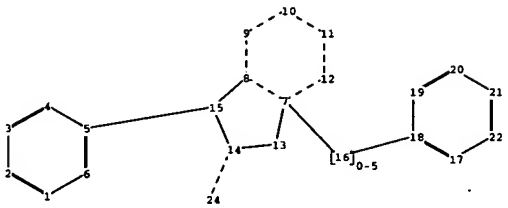
```
        27385 HEXAHYDRO
            1 HEXAHYDROS
        27386 HEXAHYDRO
                (HEXAHYDRO OR HEXAHYDROS)
         1092 BENZIMIDAZOLON?
L12         9 HEXAHYDRO AND BENZIMIDAZOLON?

=> d L12 1-9 ibib kwic

L12  ANSWER 1 OF 9  CAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2002:793608  CAPLUS
DOCUMENT NUMBER:          137:310917
TITLE:                    Aromatic-substituted thiohydantoins, their
                          preparation, and their use for treating diabetes,
                          dyslipidemia, and obesity
INVENTOR(S):              Boubia, Benaiessa; Chaput, Evelyne; Ou, Khan; Ratel,
                          Philippe
PATENT ASSIGNEE(S):       Laboratoires Fournier SA, Fr.
SOURCE:                   PCT Int. Appl., 111 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 French
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     --------------       ----   --------    --------------------     --------
     WO 2002081453         A1    20021017    WO 2002-FR1167           20020404
     WO 2002081453         C1    20021114
         W:  AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EE, EE, ES,
             FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG,
             KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW,
             MX, MZ, NO
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     FR 2823209            A1    20021011    FR 2001-4552             20010404
     FR 2823209            B1    20031212
     CA 2444024            AA    20021017    CA 2002-2444024          20020404
     EP 1373219            A1    20040102    EP 2002-730333           20020404
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     EE 200300485          A     20040216    EE 2003-485              20020404
     BR 2002007910         A     20040803    BR 2002-7910             20020404
     JP 2004525175         T2    20040819    JP 2002-579441           20020404
     ZA 2003007372         A     20040922    ZA 2003-7372             20030922
     US 2004116417         A1    20040617    US 2003-473032           20030926
     NO 2003004430         A     20031006    NO 2003-4430             20031003
PRIORITY APPLN. INFO.:                         FR 2001-4552         A  20010404
                                               WO 2002-FR1167       W  20020404

OTHER SOURCE(S):          MARPAT 137:310917
REFERENCE COUNT:          1     THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
   471938-03-1P, Ethyl 2-[[4-(4-hydroxypiperidin-1-yl)phenyl]amino]acetate
     471938-04-2P, Ethyl 2-[[4-(4-hydroxypiperidin-1-yl)phenyl]amino]propanoate
     471938-05-3P, Ethyl 2-[[4-(4-hydroxypiperidin-1-yl)phenyl]amino]butanoate
     471938-06-4P, Ethyl 2-[[4-(4-hydroxypiperidin-1-yl)phenyl]amino]pentanoate
     471938-07-5P, Ethyl 2-[[4-[4-(hydroxymethyl)piperidin-1-
     yl]phenyl]amino]acetate   471938-08-6P, Ethyl 2-[[4-[4-
     (hydroxymethyl)piperidin-1-yl]phenyl]amino]propanoate   471938-09-7P,
     Ethyl 2-[[4-[4-(hydroxymethyl)piperidin-1-yl]phenyl]amino]butanoate
     471938-10-0P, Ethyl 2-[[4-[4-(hydroxymethyl)piperidin-1-
```

C:\Program Files\Stnexp\Queries\10681924a.str

10/681,924

Structures Searched



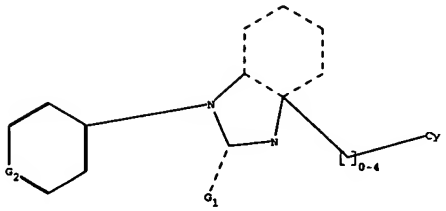


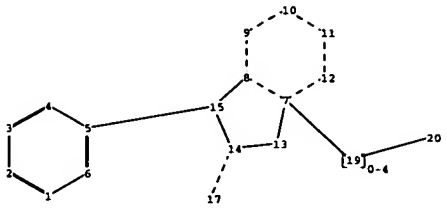
chain nodes :
16 24
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 17 18 19 20 21 22
chain bonds :
5-15 7-16 14-24 16-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14 14-15
17-18 17-22 18-19 19-20 20-21 21-22
exact/norm bonds :
5-15 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14 14-15 14-24
exact bonds :
7-16 16-18
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 24:CLASS

C:\Program Files\Stnexp\Queries\10681924b.str





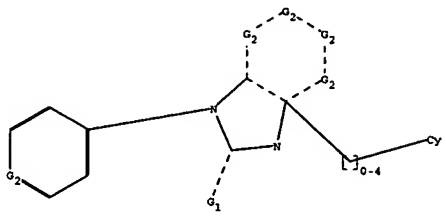
chain nodes :
17 19 20
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
5-15 7-19 14-17 19-20
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14 14-15
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-15 7-8 7-12 7-13 7-19 8-9 8-15 9-10 10-11 11-12
13-14 14-15 14-17 19-20

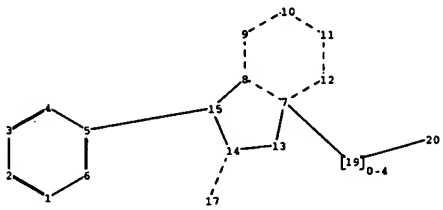
G1:O,S

G2:C,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS 19:CLASS 20:Atom

C:\Program Files\Stnexp\Queries\10681924c.str





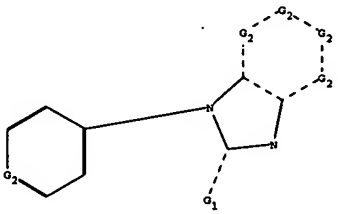
chain nodes :
17 19 20
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
5-15 7-19 14-17 19-20
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14 14-15
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-15 7-8 7-12 7-13 7-19 8-9 8-15 9-10 10-11 11-12
13-14 14-15 14-17 19-20

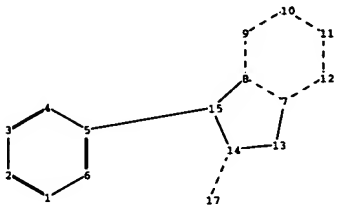
G1:O,S

G2:C,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS 19:CLASS 20:Atom

C:\Program Files\Stnexp\Queries\10681924d.str





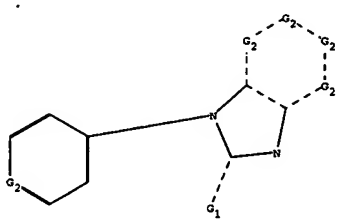
chain nodes :
17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
5-15 14-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14 14-15
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-15 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14
14-15 14-17

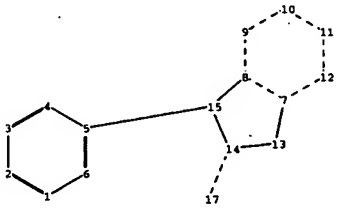
G1:O,S

G2:C,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS

C:\Program Files\Stnexp\Queries\10681924e.str





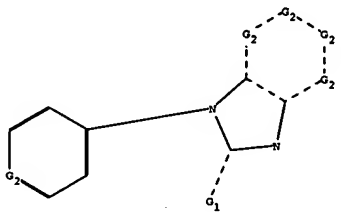
chain nodes :
17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
5-15 14-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14 14-15
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-15 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14
14-15 14-17

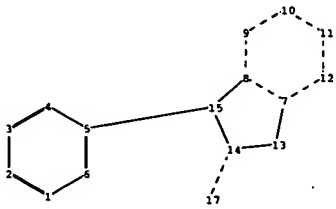
G1:O,S

G2:C,N

Hydrogen count :
7:= exact 0
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS

C:\Program Files\Stnexp\Queries\10681924f.str





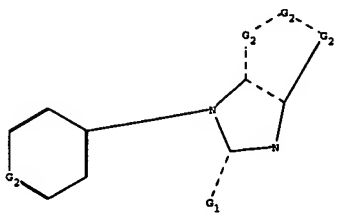
chain nodes :
17
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
chain bonds :
5-15 14-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14 14-15
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-15 7-8 7-12 7-13 8-9 8-15 9-10 10-11 11-12 13-14
14-15 14-17

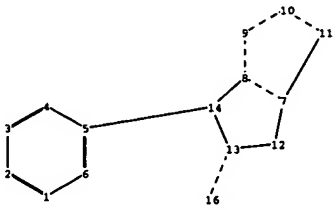
G1:O,S

G2:C,N

Hydrogen count :
7:= exact 0
Connectivity :
7:4 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS

C:\Program Files\Stnexp\Queries\10681924g.str





chain nodes :
16
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14
chain bonds :
5-14 13-16
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-11 8-9 8-14 9-10 10-11 12-13 13-14
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-14 7-8 7-12 7-11 8-9 8-14 9-10 10-11 12-13 13-14
13-16

G1:O,S

G2:C,N

Hydrogen count :
7:= exact 0
Connectivity :
7:4 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 16:CLASS